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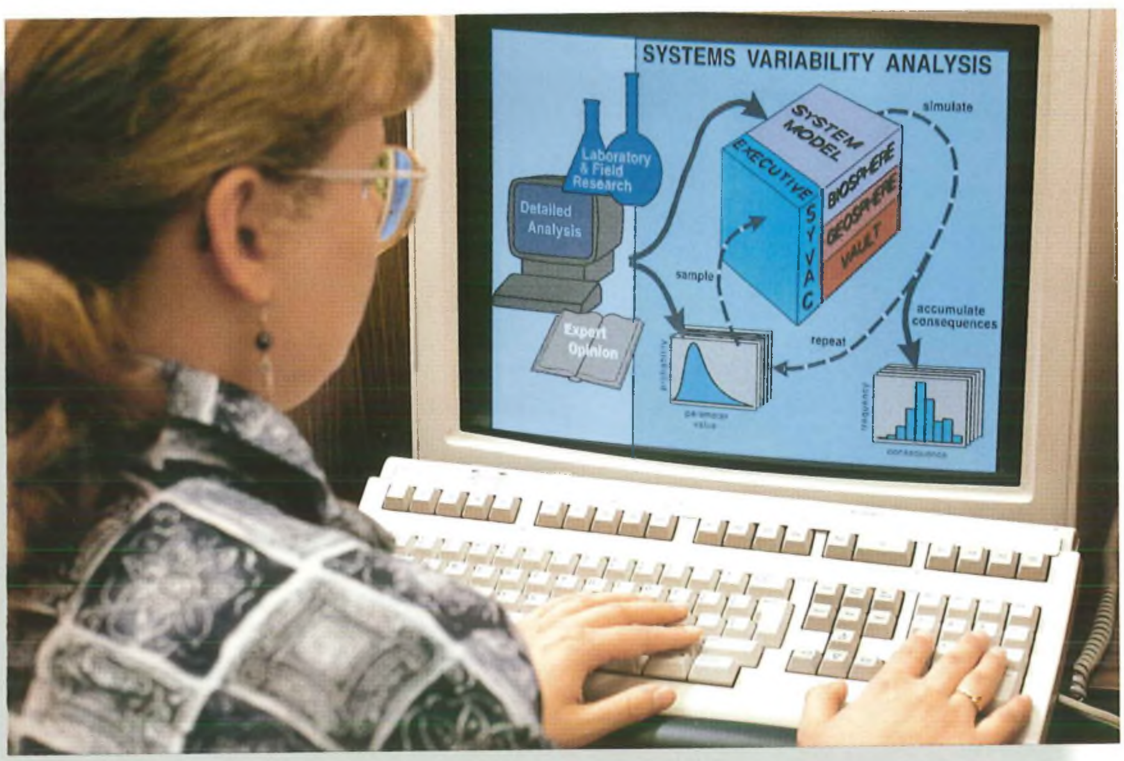
The Disposal of Canada's Nuclear Fuel Waste: Postclosure Assessment of a Reference System

Le stockage permanent des déchets de combustible nucléaire du Canada : Évaluation de post-fermeture d'un système de référence

B.W. Goodwin, D.B. McConnell, T.H. Andres, W.C. Hajas, D.M. LeNeveu, T.W. Melnyk, G.R. Sherman, M.E. Stephens, J.G. Szekely, P.C. Bera, C.M. Cosgrove, K.D. Dougan, S.B. Keeling, C.I. Kitson, B.C. Kummen, S.E. Oliver, K. Witzke, L. Wojciechowski, A.G. Wikjord



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AECL RESEARCH

THE DISPOSAL OF CANADA'S NUCLEAR FUEL WASTE: POSTCLOSURE ASSESSMENT OF A REFERENCE SYSTEM

by

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Whiteshell Laboratories
Pinawa, Manitoba R0E 1L0
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ABSTRACT

The concept for disposal of Canada's nuclear fuel waste is based on a vault located deep in plutonic rock of the Canadian Shield.

We document in this report a method to assess the long-term impacts of a disposal facility for nuclear fuel waste. The assessment integrates relevant information from engineering design studies, site investigations, laboratory studies, expert judgment and detailed mathematical analyses to evaluate system performance in terms of safety criteria, guidelines and standards. The method includes the use of quantitative tools such as the SYstems Variability Analysis computer Code (SYVAC) to deal with parameter uncertainty and the use of reasoned arguments based on well-established scientific principles.

We also document the utility of the method by describing its application to a hypothetical implementation of the concept called the reference disposal system. The reference disposal system generally conforms to the overall characteristics of the concept, except we have made some specific site and design choices so that the assessment would be more realistic. To make the reference system more representative of a real system, we have used the geological observations of the AECL's Whiteshell Research Area located near Lac du Bonnet, Manitoba, to define the characteristics of the geosphere and the groundwater flow system. This research area has been subject to more than a decade of geological and hydrological studies.

The analysis of the reference disposal system provides estimates of radiological and chemical toxicity impacts on members of a critical group and estimates of possible impacts on the environment. The latter impacts include estimates of radiation dose to nonhuman organisms. Other quantitative analyses examine the use of derived constraints to improve the margin of safety, the effectiveness of engineered and natural barriers, and the sensitivity of the results to influential features, events, and processes of the reference disposal system.

The study results indicate that the reference disposal system would meet the requirements established by the Atomic Energy Control Board and indicate that implementation of the disposal concept can provide safe disposal of nuclear fuel waste using currently available or readily achievable technology and without relying on institutional controls to maintain safety in the long term.

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LE STOCKAGE PERMANENT DES DÉCHETS DE COMBUSTIBLE NUCLÉAIRE DU CANADA : ÉVALUATION DE POST-FERMETURE D'UN SYSTÈME DE RÉFÉRENCE

par

B.W. Goodwin, D.B. McConnell, T.H. Andres, W.C. Hajas, D.M. LeNeveu, T.W. Melnyk, G.R. Sherman, M.E. Stephens, J.G. Szekely, P.C. Bera C.M. Cosgrove, K.D. Dougan, S.B. Keeling, C.I. Kitson, B.C. Kummen, S.E. Oliver, K. Witzke, L. Wojciechoski et A.G. Wikjord

RÉSUMÉ

Le concept de stockage permanent des déchets de combustible nucléaire du Canada est basé sur une installation souterraine située à grande profondeur dans la roche plutonique du Bouclier canadien.

Dans le présent rapport, nous documentons une méthode d'évaluation des impacts à long terme d'une installation de stockage permanent des déchets de combustible nucléaire. L'évaluation intègre les renseignements pertinents provenant d'études de plans techniques, d'études de sites, d'études en laboratoire, d'opinion d'experts et d'analyses mathématiques précises pour évaluer le fonctionnement et comportement quant aux critères de sûreté, directives et normes. La méthode comprend l'utilisation d'outils d'analyse quantitative tels que le Programme d'analyse de variabilité des systèmes (SYVAC) pour pallier à l'incertitude des paramètres et l'emploi d'arguments raisonnés basé sur des principes scientifiques bien établis.

Nous documentons également l'utilité de la méthode en décrivant son application à une mise en pratique hypothétique du concept appelée le système de stockage permanent de référence. Le système de stockage permanent de référence se conforme généralement aux caractéristiques générales du concept, à part que nous avons choisi un site et un plan particuliers de telle sorte que l'évaluation soit plus réaliste. Pour rendre le système de référence plus représentatif d'un système réel, nous nous sommes servis des observations géologiques de l'Aire de recherches de Whiteshell d'EACL, laquelle est située près de Lac du Bonnet au Manitoba, pour définir les caractéristiques de la géosphère et du réseau d'écoulement d'eaux souterraines. Cette aire de recherches a été l'objet d'études géologiques et hydrologiques s'étendant sur plus d'une décennie.

L'analyse du système de stockage permanent de référence permet de fournir des valeurs estimées des impacts radiologique et chimique sur les personnes d'un groupe critique et des valeurs estimées d'impacts possibles sur l'environnement. Ces dernières comprennent les valeurs estimées de la dose de rayonnement aux organismes non humains. D'autres analyses quantitatives permettent d'examiner l'emploi de contraintes dérivées pour améliorer la marge de sécurité, l'efficacité des barrières ouvragées et naturelles et la sensibilité des résultats aux caractéristiques, événements et processus influents du système de stockage permanent de référence.

Les résultats de l'étude indiquent que le système de stockage permanent de référence satisferait aux conditions établies par la Commission de contrôle de l'énergie atomique, et que la mise en pratique du concept de stockage permanent peut assurer le stockage permanent sûr des déchets de combustible nucléaire à l'aide de techniques existant actuellement ou facilement réalisables et sans se reposer sur le contrôle institutionnel pour maintenir la sûreté à long terme.

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PREFACE

In 1992, 15% of the electricity generated in Canada was produced using CANDU nuclear reactors. A by-product of the nuclear power is used CANDU fuel, which consists of ceramic uranium dioxide pellets and metal structural components. Used fuel is highly radioactive. The used fuel from Canada's power reactors is currently stored in water-filled pools or dry storage concrete containers. Humans and other living organisms are protected by isolating the used fuel from the natural environment and by surrounding it with shielding material. Current storage practices have an excellent safety record.

At present, used CANDU fuel is not reprocessed. It could, however, be reprocessed to extract useful material for recycling, and the highly radioactive material that remained could be incorporated into a solid. The term "nuclear fuel waste," as used by AECL, refers to either

- the used fuel, if it is not reprocessed, or

- a solid incorporating the highly radioactive waste from reprocessing.

Current storage practices, while safe, require continuing institutional controls such as security measures, monitoring, and maintenance. Thus storage is an effective interim measure for protection of human health and the natural environment but not a permanent solution. A permanent solution is disposal, a method "in which there is no intention of retrieval and which, ideally, uses techniques and designs that do not rely for their success on long-term institutional control beyond a reasonable period of time" (AECB 1987).

In 1978, the governments of Canada and Ontario established the Nuclear Fuel Waste Management Program "to assure the safe and permanent disposal" of nuclear fuel waste. AECL was made responsible for research and development on "disposal in a deep underground repository in intrusive igneous rock" (Joint Statement 1978). Ontario Hydro was made responsible for studies on interim storage and transportation of used fuel and has contributed to the research and development on disposal. Over the years a number of other organizations have also contributed to the Program, including Energy, Mines and Resources Canada; Environment Canada; universities; and companies in the private sector.

The disposal concept is to place the waste in long-lived containers; emplace the containers, enveloped by sealing materials, in a disposal vault excavated at a nominal depth of 500 to 1000 m in intrusive igneous (plutonic) rock of the Canadian Shield; and (eventually) seal all excavated openings and exploration boreholes to form a passively safe system. Thus there would be multiple barriers to protect humans and the natural environment from contaminants in the waste: the container, the very low-solubility waste form, the vault seals, and the geosphere. The disposal technology includes options for the design of the engineered components, including the disposal container, disposal vault, and vault seals, so that it is adaptable to a wide range of regulatory standards, physical conditions, and social requirements. Potentially suitable bodies of plutonic rock occur in a large number of locations across the Canadian Shield.

In developing and assessing this disposal concept, AECL has consulted broadly with members of Canadian society to help ensure that the concept and the way in which it would be implemented are technically sound and represent a generally acceptable disposal strategy. Many groups in Canada have had opportunities to comment on the disposal concept and on the waste management program. These include government departments and agencies, scientists, engineers, sociologists, ethicists, and other members of the public. The Technical Advisory Committee to AECL on the Nuclear Fuel Waste Management Program, whose members are nominated by Canadian scientific and engineering societies, has been a major source of technical advice.

In 1981, the governments of Canada and Ontario announced that "... no disposal site selection will be undertaken until after the concept has been accepted. This decision also means that the responsibility for disposal site selection and subsequent operation need not be allocated until after concept acceptance" (Joint Statement 1981).

The acceptability of the disposal concept is now being reviewed by a federal Environmental Assessment Panel, which is also responsible for examining a broad range of issues related to nuclear fuel waste management (Minister of the Environment, Canada 1989). After consulting the public, the Panel issued guidelines to identify the information that should be provided by AECL, the proponent of the disposal concept (Federal Environmental Assessment Review Panel 1992).

AECL is preparing an Environmental Impact Statement to provide information requested by the Panel and to present AECL's case for the acceptability of the disposal concept. A Summary will be issued separately. This report is one of nine primary references that summarize major aspects of the disposal concept and supplement the information in the Environmental Impact Statement. A guide to the contents of the Environmental Impact Statement, the Summary, and the primary references follows this Preface.

In accordance with the 1981 Joint Statement of the governments of Canada and Ontario, no site for disposal of nuclear fuel waste is proposed at this time. Thus in developing and assessing the disposal concept, AECL could not design a facility for a proposed site and assess the environmental effects to determine the suitability of the design and the site, as would normally be done for an Environmental Impact Statement. Instead, AECL and Ontario Hydro have specified illustrative "reference" disposal systems and assessed those.

A "reference" disposal system illustrates what a disposal system, including the geosphere and biosphere, might be like. Although it is hypothetical, it is based on information derived from extensive laboratory and field research. Many of the assumptions made are conservative, that is, they would tend to overestimate adverse effects. The technology specified is either available or judged to be readily achievable. A reference disposal system includes one possible choice among the options for such things as the waste form, the disposal container, the vault layout, the vault seals, and the system for transporting nuclear fuel waste to a disposal facility.

The components and designs chosen are not presented as ones that are being recommended but rather as ones that illustrate a technically feasible way of implementing the disposal concept.

After the Panel has received the requested information, it will hold public hearings. It will also consider the findings of the Scientific Review Group, which it established to provide a scientific evaluation of the disposal concept. According to the Panel's terms of reference "As a result of this review the Panel will make recommendations to assist the governments of Canada and Ontario in reaching decisions on the acceptability of the disposal concept and on the steps that must be taken to ensure the safe long-term management of nuclear fuel wastes in Canada" (Minister of the Environment, Canada 1989).

Acceptance of the disposal concept at this time would not imply approval of any particular site or facility. If the disposal concept is accepted and implemented, a disposal site would be sought, a disposal facility would be designed specifically for the site that was proposed, and the potential environmental effects of the facility at the proposed site would be assessed. Approvals would be sought in incremental stages, so concept implementation would entail a series of decisions to proceed. Decision-making would be shared by a variety of participants, including the public. In all such decisions, however, safety would be the paramount consideration.

The EIS, Summary, and Primary References

Environmental Impact Statement on the Concept for Disposal of Canada's Nuclear Fuel Waste (AECL 1994a)
Summary of the Environmental Impact Statement on the Concept for Disposal of Canada's Nuclear Fuel Waste (AECL 1994b)
The Disposal of Canada's Nuclear Fuel Waste: Public Involvement and Social Aspects (Greber et al. 1994)
The Disposal of Canada's Nuclear Fuel Waste: Site Screening and Site Evaluation Technology (Davison et al. 1994a)
The Disposal of Canada's Nuclear Fuel Waste: Engineered Barriers Alternatives (Johnson et al. 1994b)
The Disposal of Canada's Nuclear Fuel Waste: Engineering for a Disposal Facility (Simmons and Baumgartner 1994)
The Disposal of Canada's Nuclear Fuel Waste: Preclosure Assessment of a Conceptual System (Grondin et al. 1994)
The Disposal of Canada's Nuclear Fuel Waste: Postclosure Assessment of a Reference System (Goodwin et al. 1994)
The Disposal of Canada's Nuclear Fuel Waste: The Vault Model for Postclosure Assessment (Johnson et al. 1994a)
The Disposal of Canada's Nuclear Fuel Waste: The Geosphere Model for Postclosure Assessment (Davison et al. 1994b)
The Disposal of Canada's Nuclear Fuel Waste: The Biosphere Model, BIOTRAC, for Postclosure Assessment (Davis et al. 1993)

GUIDE TO THE CONTENTS OF THE ENVIRONMENTAL IMPACT STATEMENT, THE SUMMARY, AND THE PRIMARY REFERENCES

ENVIRONMENTAL IMPACT STATEMENT AND SUMMARY

Environmental Impact Statement on the Concept for Disposal of Canada's Nuclear Fuel Waste (AECL 1994a)

- provides an overview of AECL's case for the acceptability of the disposal concept
- provides information about the following topics:
  - the characteristics of nuclear fuel waste
  - storage and the rationale for disposal
  - major issues in nuclear fuel waste management
  - the disposal concept and implementation activities
  - alternatives to the disposal concept
  - methods and results of the environmental assessments
  - principles and potential measures for managing environmental effects
  - AECL's overall evaluation of the disposal concept

Summary of the Environmental Impact Statement on the Concept for Disposal of Canada's Nuclear Fuel Waste (AECL 1994b)

- summarizes the contents of the Environmental Impact Statement

PRIMARY REFERENCES

The Disposal of Canada's Nuclear Fuel Waste: Public Involvement and Social Aspects (Greber et al. 1994)

- describes the activities undertaken to provide information to the public about the Nuclear Fuel Waste Management Program and to obtain public input into the development of the disposal concept
- presents the issues raised by the public and how the issues have been addressed during the development of the disposal concept or how they could be addressed during the implementation of the disposal concept
- discusses social aspects of public perspectives on risk, ethical issues associated with nuclear fuel waste management, and principles for the development of a publicly acceptable site selection process

The Disposal of Canada's Nuclear Fuel Waste: Site Screening and Site Evaluation Technology (Davison et al. 1994a)

- discusses geoscience, environmental, and engineering factors that would need to be considered during siting

- describes the methodology for characterization, that is, for obtaining the data about regions, areas, and sites that would be needed for facility design, monitoring, and environmental assessment

The Disposal of Canada's Nuclear Fuel Waste: Engineered Barriers Alternatives (Johnson et al. 1994a)

- describes the characteristics of nuclear fuel waste

- describes the materials that were evaluated for use in engineered barriers, such as containers and vault seals

- describes potential designs for containers and vault seals

- describes procedures and processes that could be used in the production of containers and the emplacement of vault-sealing materials

The Disposal of Canada's Nuclear Fuel Waste: Engineering for a Disposal Facility (Simmons and Baumgartner 1994)

- discusses alternative vault designs and general considerations for engineering a nuclear fuel waste disposal facility

- describes a disposal facility design that was used to assess the technical feasibility, costs, and potential effects of disposal (Different disposal facility designs are possible and might be favoured during concept implementation.)

- presents cost and labour estimates for implementing the design

The Disposal of Canada's Nuclear Fuel Waste: Preclosure Assessment of a Conceptual System (Grondin et al. 1994)

- describes a methodology for estimating effects on human health, the natural environment, and the socio-economic environment that could be associated with siting, constructing, operating (includes transporting used fuel), decommissioning, and closing a disposal facility

- describes an application of this assessment methodology to a reference disposal system (We use the term "reference" to designate the disposal systems, including the facility designs, specified for the assessment studies. Different disposal facility designs are possible and might be favoured during concept implementation.)

- discusses technical and social factors that would need to be considered during siting

- discusses possible measures and approaches for managing environmental effects

The Disposal of Canada's Nuclear Fuel Waste: Postclosure Assessment of a Reference System (Goodwin et al. this volume)

- describes a methodology for
  - estimating the long-term effects of a disposal facility on human health and the natural environment,
  - determining how sensitive the estimated effects are to variations in site characteristics, design parameters, and other factors, and
  - evaluating design constraints

- describes an application of this assessment methodology to a reference disposal system (We use the term "reference" to designate the disposal systems, including the facility designs, specified for the assessment studies. Different disposal facility designs are possible and might be favoured during concept implementation.)

The Disposal of Canada's Nuclear Fuel Waste: The Vault Model for Postclosure Assessment (Johnson et al. 1994b)

- describes the assumptions, data, and model used in the postclosure assessment to analyze processes within and near the buried containers of waste

- discusses the reliability of the data and model

The Disposal of Canada's Nuclear Fuel Waste: The Geosphere Model for Postclosure Assessment (Davison et al. 1994b)

- describes the assumptions, data, and models used in the postclosure assessment to analyze processes within the rock in which a disposal vault is excavated

- discusses the reliability of the data and model

The Disposal of Canada's Nuclear Fuel Waste: The Biosphere Model, BIOTRAC, for Postclosure Assessment (Davis et al. 1993)

- describes the assumptions, data, and model used in the postclosure assessment to analyze processes in the near-surface and surface environment

- discusses the reliability of the data and model

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EXECUTIVE SUMMARY

ES.1 INTRODUCTION

Context of This Report

AECL Research is submitting for public review an Environmental Impact Statement (EIS) for the disposal of Canada's nuclear fuel waste. The EIS (AECL 1994a) is supported by nine primary references identified in the preface.

Two of these primary references present assessments of the potential impacts of a conceptual facility on the public, workers and the environment.

- The *preclosure assessment* (Grondin et al. 1994) deals with environmental and safety issues that may arise during the facility construction, operation, decommissioning and extended monitoring stages, prior to and including closure of the disposal facility.

- The *postclosure assessment*, documented in this report, deals with long-term environmental and safety issues. The time frame of concern for the postclosure assessment begins after the disposal facility has been closed and all shafts, tunnels and boreholes have been sealed, so that the facility is placed in a passively safe state. The postclosure phase also extends indefinitely into the future.

If the concept were accepted, implementation of an actual facility would proceed through stages that include siting, construction, operation, decommissioning, extended monitoring and closure (AECL 1994a), and postclosure assessments would be performed during each of these stages. It is our view that postclosure assessment would play a significant role throughout implementation, by providing information that is essential for decision making. In particular, assessments conducted at each stage and substage of the project would contribute to the rationale and justification to continue to the next step. Eventually, postclosure assessment would contribute toward a decision on closure of the facility.

The application of the postclosure assessment described in this document is approximately equivalent to interim investigations that would be conducted during the siting stage for the evaluation of a potential site. In particular, this document describes the analysis that could be performed at a time when there is substantial information from studies on the surface and in exploration boreholes, but prior to exploratory excavation. Thus the primary purpose of this assessment would be to contribute toward decisions on whether to begin exploratory excavation at the site in question, so as to permit a more complete evaluation of its technical merits. Subsequent postclosure assessments of this site, and similar assessments of other potential sites, would contribute to selecting a preferred site and to obtaining approvals for the construction of a disposal facility at that site.

Objectives of the Postclosure Assessment

The principal objectives of the postclosure assessment are to

- develop and document a method for estimating and evaluating the long-term effects and safety of a facility for the disposal of Canada's nuclear fuel waste; and

- demonstrate the utility of this method by applying it to a hypothetical implementation of the concept, which we refer to as the reference disposal system.

In demonstrating the method, specific objectives of the postclosure assessment of the reference disposal system are to

- identify possible long-term environmental and safety impacts, notably radiation dose to individuals most at risk, and estimate the magnitudes of the impacts;

- compare the magnitudes of these estimated impacts with safety criteria established by regulatory agencies in Canada; and

- conduct sensitivity analyses to identify factors that could have a large influence on the number and magnitude of potential impacts.

Our postclosure assessment uses deterministic and probabilistic methods to evaluate impacts. The deterministic methodology provides detailed insight into the operation of the disposal system, whereas the probabilistic assessment methodology provides a comprehensive and systematic approach to account for uncertainty. The analyses are focussed on possible environmental and safety impacts, such as radiation dose to people who would be most at risk, radiation dose to other biota and concentrations of contaminants in the soil, water and air in the vicinity of a disposal facility. (We use the term contaminants to refer to both radioactive and nonradioactive nuclides from the nuclear fuel waste.) We also estimate the radiological risk for comparison with regulatory criteria by applying a prescribed risk equation (AECB 1987a). Radiological risk is a measure of the probability of serious health effects per year that may result from the disposal system.

The postclosure assessment described in this report is applied to a hypothetical disposal system, and not to a specific project. Thus the results of the analysis should be interpreted with appropriate qualifications and used with caution.

Scope of the Postclosure Assessment

The concept for the disposal of Canada's nuclear fuel waste involves deep underground burial in a vault excavated in plutonic rock of the Canadian Shield (AECL 1994a,b). A series of engineered and natural barriers would immobilize and isolate the waste.

The features of the concept relevant to the postclosure assessment concern the long-term behaviour of the waste after the rooms in the vault would have been filled, the access tunnels and shafts would have been sealed, and the surface facilities would have been removed. The postclosure assessment is concerned with the entire disposal system: the disposal vault itself and the surrounding geosphere and biosphere that might be affected by the presence of the disposal vault.

To provide quantitative estimates of impacts, the postclosure assessment uses mathematical simulations to study the behaviour of contaminants in the disposal system. The simulations are based on defensible scientific principles, using current information and knowledge to construct a system model that represents the disposal system. We then interrogate the system model to evaluate future behaviour. The system model does not predict in detail the actual future of the disposal system. Rather it provides an estimate of impacts that will not be exceeded; that is, it overestimates impacts. This a common practice in safety analysis.

For times far into the distant future, we also use reasoned arguments that are based on the geological record and well-established scientific principles.

Environmental Criteria, Guidelines and Standards

In Canada, the Atomic Energy Control Board (AECB) is responsible for the regulations for the licensing and operation of nuclear facilities. The AECB has issued three regulatory documents that apply to the postclosure assessment: R-71 (AECB 1985) outlines the AECB's general requirements for a regulatory review and assessment of the concept; R-104 (AECB 1987a) provides quantitative and qualitative regulatory objectives, requirements and guidelines for judging the acceptability of the long-term performance of radioactive waste disposal options; and R-72 (AECB 1987b) discusses fundamental objectives and requirements for siting a disposal facility. The AECB Regulatory Document R-104 includes a radiological risk limit that is calculated from estimates of annual dose.

We use the term annual dose (to humans) as an abbreviation for annual effective dose equivalent, and we report it in units of sieverts per year (Sv/a). Annual dose determines the biological consequences of internal and external exposures to ionizing radiation, with corrections accounting for the effectiveness of different types of radiation in causing biological effects and the radiosensitivity of different body organs. The internal exposures are 50-year committed effective dose equivalents, meaning that they account for radiation dose received during the current year, plus the dose that would be received over the next 49 years from those radioactive contaminants that may remain in the human body. We calculate annual dose for members of a hypothetical group of individuals, called the critical group, who are expected to be most at risk from the disposal system.

The AECB Regulatory Documents R-71 and R-104 (AECB 1985, 1987a) also specify that environmental impacts must be assessed for nonradioactive contaminants released from the disposal facility, although no specific requirements are provided. We use criteria based on available Canadian regulations and guidelines, such as guidelines for drinking water and for cleanup of contaminated soil. Guidelines are not established for some contaminants, and for these contaminants we have assumed stringent guidelines to identify contaminants of concern. We then evaluate their potential to cause a significant effect.

Finally, there is a more general requirement for protection of the environment that is discussed in R-104 AECB (1987a) and in the guidelines from the Environmental Assessment and Review Panel (EARP 1992). We examine possible effects on the environment attributed to the presence of a disposal vault. These effects include an estimate of concentrations of all radioactive and nonradioactive contaminants in soil and water, and then a comparison of these concentrations with environmental baseline data from the Canadian Shield. We use this exacting test to identify contaminants of potential concern for protection of the environment. For the contaminants of concern, we focus our analysis on how and to what extent they could affect the environment. A key part of the analysis is an evaluation of the effects of estimated radiation doses to nonhuman organisms.

ES.2 THE ASSESSMENT METHOD

The approach we use conforms to the objectives, scope and regulatory requirements described above. Because the disposal system is designed to protect humans and the environment for tens of thousands of years, we cannot base the quantitative assessment on observations of its long-term performance. We have, therefore, adopted a simulation approach, using mathematical models to infer the long-term behaviour of a disposal system and to estimate its potential effects. We describe the assessment approach using the six steps shown in Figure ES-1 and note there is considerable feedback among the steps.

1. Specify the System Features

The concept for disposal of Canada's nuclear fuel waste is based upon emplacement in plutonic rock of the Canadian Shield. A complete description of the concept, including a number of design options, is provided in the EIS (AECL 1994a) and in the primary references describing the engineered barriers (Johnson et al. 1994a) and the conceptual design (Simmons and Baumgartner 1994).

The reference disposal system assessed in this report generally conforms with the characteristics of the concept, although it considers some specific assumptions and design choices; for example, the disposal vault is located at a depth of 500 m, the nuclear waste is used-fuel bundles containing irradiated uranium dioxide fuel and Zircaloy sheaths, the used-fuel bundles are placed in thin-walled containers constructed from Grade-2 titanium, the containers are emplaced in boreholes in the floor of the rooms of the disposal vault, a swelling clay (called the buffer) isolates the containers in the boreholes from the surrounding rock, and the vault is located within a particular geosphere for which a reasonably complete set of environmental and geological data are available. Figure ES-2 illustrates some of the features of the reference disposal system.

EIS 6 ES-1

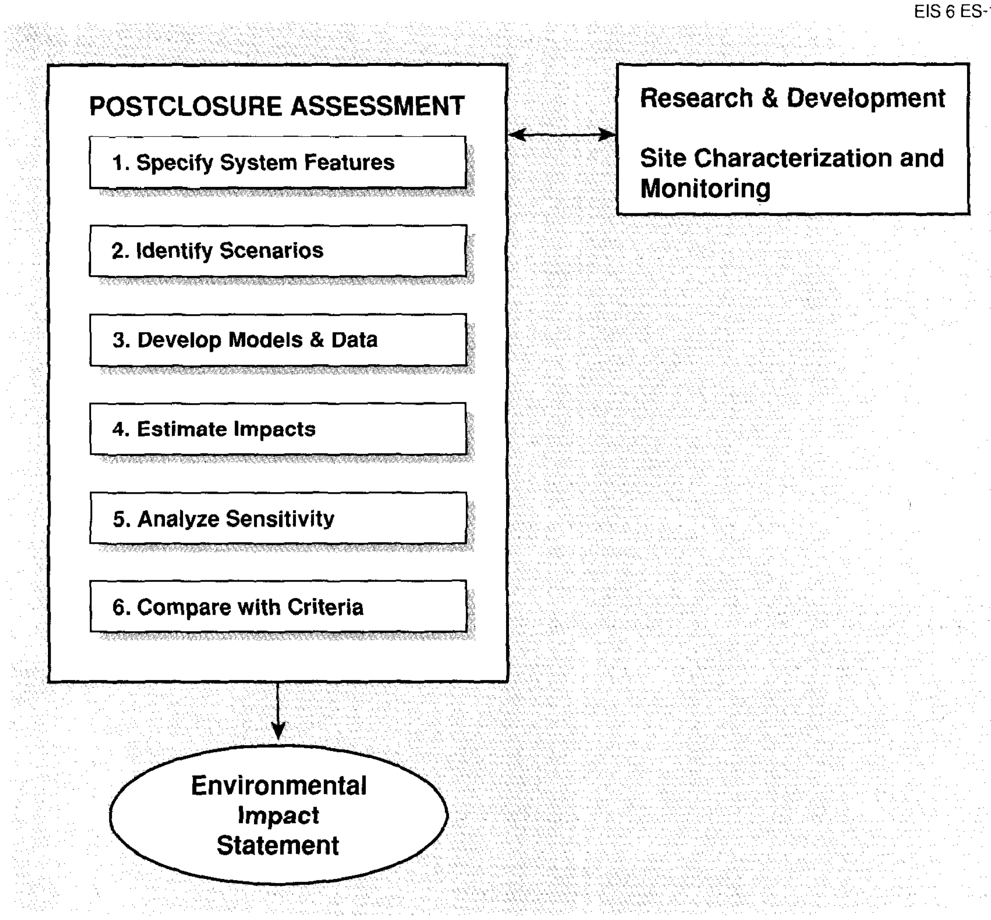

FIGURE ES-1: Overview of the Steps in the Postclosure Assessment

Not shown is the feedback in which the results and conclusions from one step may bring about some changes in one or more other steps. For example, preliminary estimates of impacts and comparisons with criteria can lead to changes in the system features and to other steps in the assessment.

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2. Identify Scenarios

In this step, we systematically search for all factors that could affect the future performance of the reference disposal system. Examples of such factors are container corrosion, diffusion of contaminants in groundwater, movement of groundwater and contaminants in the geosphere including movement along fracture zones, and the use of wells to supply drinking water. We then assemble the factors into scenarios, or combinations of factors, for detailed assessment. For the study described in this report, we concluded that three types of scenarios require quantitative evaluation.

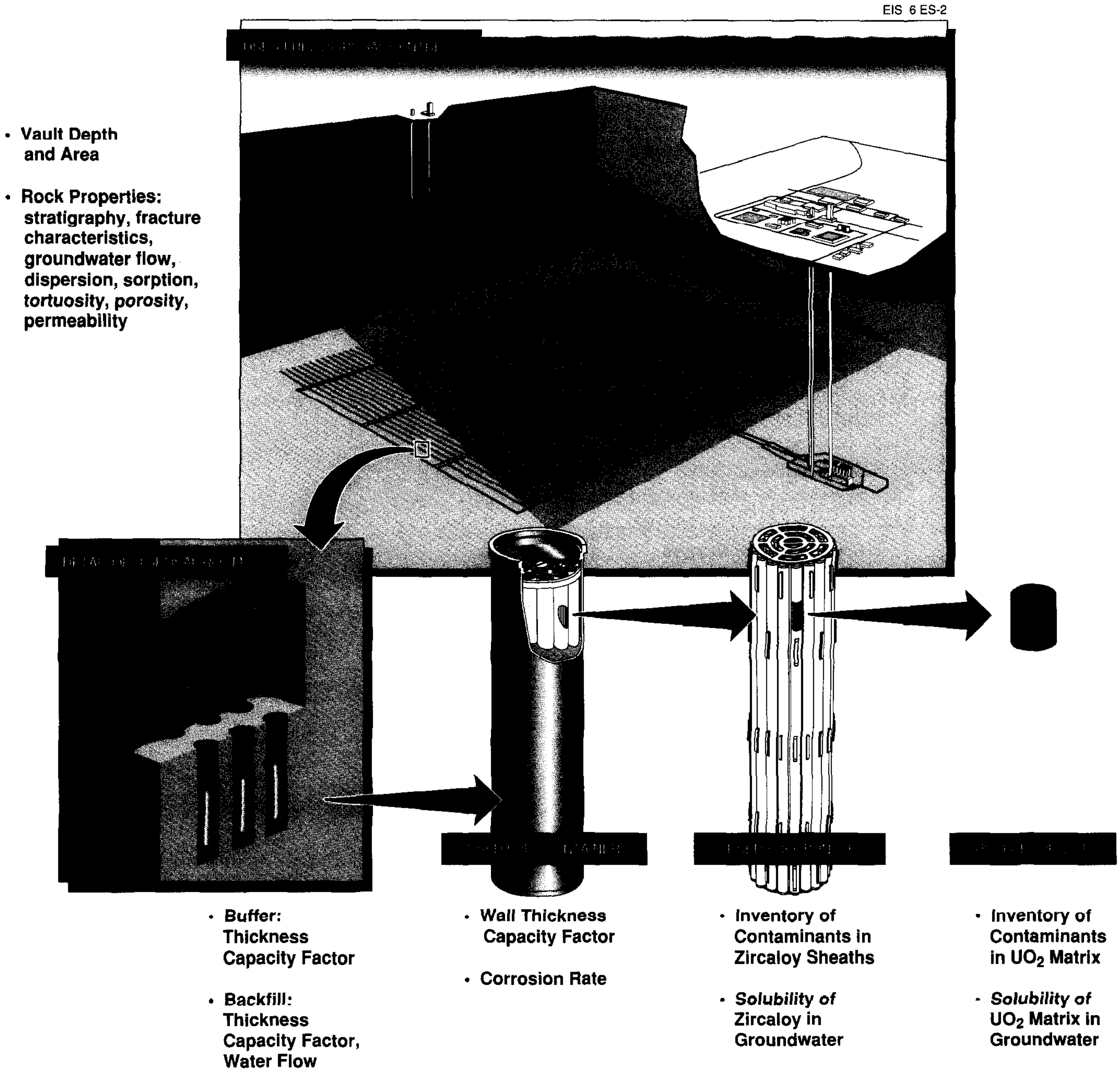

FIGURE ES-2: Some Features of the Reference Disposal System

This figure illustrates the different scales of engineered and natural barriers in the reference disposal system and lists some of their properties that are important.

The first type of scenarios contains most of the identified factors. They are called the SYVAC scenarios because they are evaluated using the SYstems Variability Analysis Code (or SYVAC). For the assessment of the reference disposal system, we conservatively assume the total probability associated with the SYVAC scenarios is unity. These scenarios deal with groundwater-mediated processes: corrosion of the containers, dissolution of the waste, release of contaminants from the vault, transport of contaminants through the geosphere and the biosphere, where they may cause impacts to humans, to other biota and to the environment. The SYVAC scenarios include many scenarios; for example, they include situations where a well or a lake supplies the drinking water used by the critical group, and situations where crops are grown on different types of soil or on lake sediment.

The second type of scenarios requiring detailed evaluation for the reference disposal system is known as the open-borehole scenarios. These scenarios deal with the unlikely possibility that one or more deep boreholes may remain open after closure of the disposal vault and provide important transport pathways for contaminants in the disposal vault.

The third type of scenarios deals with disruptive events that could seriously impair the integrity of a disposal system. For the reference disposal system, we conclude that one such event requires detailed evaluation: inadvertent human intrusion, in which the intruder is unaware of the existence of the disposal vault and the hazard that it presents. We assume these scenarios are initiated by a low-probability event in which a deep exploration borehole is drilled through a container in the vault, and nuclear fuel waste is brought directly to the surface environment.

3. Develop Models and Data for Simulating the System

In step 3, we gather together all the available information and data required to describe the scenarios requiring evaluation.

We construct mathematical models to simulate how contaminants could move throughout the reference disposal system. In constructing these models, we first relate observed data to our understanding of geology, physics, chemistry, biology, health sciences and other disciplines. We then represent these observations and understanding using mathematical models that describe the known data and that can be used to describe future behaviour. A key challenge in constructing these models is ensuring that they are appropriate for their intended use, which is to evaluate the long-term performance and safety of the disposal system and to provide estimates of potential impacts that would not be exceeded. The system model developed for the SYVAC scenarios is described in detail in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993). These primary references include discussion of the assumptions made in constructing the models and justification of the data used in the models.

The models contain parameters that represent the important features of the system. Figure ES-2 gives examples of these parameters, such as the inventory of contaminants in the UO_2 matrix. The value selected for a parameter reflects the observations and measurements from field and laboratory studies. In many cases, it may not be feasible to provide a *single precise* value for a parameter and, therefore, we allow for ranges of possible parameter values. For each parameter, the range and weighting of different possible values are specified using a probability density function (PDF) assigned by qualified experts in appropriate scientific and engineering disciplines. The experts select an appropriate PDF to account for the uncertainty in possible parameter values, including uncertainty arising from natural variability and the current state of knowledge.

In constructing these models and specifying their associated parameter values, we have made a number of conservative assumptions. That is, where it is not necessary or possible to be realistic, we have introduced assumptions that would lead to overestimates of impacts.

4. Estimate Impacts

We use the models and data to simulate the long-term behaviour of contaminants in the reference disposal system and to provide (over)estimates of impact. For quantitative studies of the SYVAC scenarios, we performed both a deterministic analysis and a probabilistic analysis, using the computer program SYVAC3-CC3 (SYstems Variability Analysis Code generation 3, with models for the Canadian Concept, version 3). These two analyses provide complementary information.

- *Deterministic analysis* provides insights into how and where contaminants move within the system. Our analyses are focussed on the *median-value simulation*, named thus because it uses the median value for each parameter. The median value is a central value from the range of possible values (more precisely, it is the value corresponding to the 50^{th} percentile of the parameter PDF).

- *Probabilistic analysis* takes into account the effects of uncertainty and variability in parameters used by the system model. In this analysis, we use the results from thousands of simulations, each having a different set of randomly sampled values for all parameters. The values are sampled from the PDFs associated with the parameters. To compare the estimates of impact with regulatory criteria, we use the arithmetic average (or mean) of the estimates from the large set of simulations. Use of the arithmetic average is prescribed in the AECB *Regulatory Document* R-104 (AECB 1987a). The arithmetic average of an impact corresponds to its (mathematical) expectation value, taking into account the effects of uncertainty in the values of the parameters.

The deterministic (or median-value) and probabilistic analyses for the SYVAC scenarios cover the period of time from closure of the disposal facility up to 10^5 a into the future. Results of the analyses, outlined in Section ES.3, include estimates for variables such as annual dose to humans and to nonhuman biota, and concentrations of contaminants in soil and water.

We also describe in Section ES.3 our analyses of the open-borehole and inadvertent human intrusion scenarios.

Reasoned arguments to extend the analyses of potential effects to longer time frames are outlined in Section ES.4.

5. Analyze the Sensitivity of the System

In sensitivity analysis, we systematically vary parameter values and observe the changes in the estimated impacts to improve our understanding of the importance of different factors on the performance of the disposal system. We are especially interested in identifying those parameters that have the greatest effect on the frequency, magnitude and variability of potential impacts.

Our study of the SYVAC scenarios for the reference disposal system includes sensitivity analyses of both the median-value and probabilistic results. We also document a preliminary study to identify potential derived constraints for the disposal system. A derived constraint is a siting or engineering restriction that might be imposed so that a disposal system would better comply with regulatory criteria and provide a greater margin of safety. We applied one such constraint, pertaining to the separation of the reference disposal vault from a nearby geological feature (referred to as fracture zone LD1), in developing a final description of the reference disposal system.

6. Compare Estimated Impacts with Regulatory Criteria

Finally, we compare estimated impacts with regulatory criteria. Our discussion in Section ES.5 summarizes the results of the analysis for the reference disposal system for the SYVAC, open-borehole and human intrusion scenarios. There are two main parts to the summary.

- The first deals with times up to 10^4 a. We use the results from Section ES.3 to estimate the total radiological risk from all significant scenarios for comparison with the AECB (1987a) radiological risk criterion.

- The second deals with times beyond 10^4 a. The AECB criteria (AECB 1987a) require that, if estimates of annual dose do not peak within 10^4 a, "there must be reasoned argument leading to the conclusion that beyond 10 000 years sudden and dramatic increases in the rate of release [of radionuclides] to the environment will not occur, acute doses will not be encountered by individuals and that major impacts will not be imposed on the biosphere". We provide some specific arguments in Section ES.4, and more general arguments in the EIS (AECL 1994a) and in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993).

ES.3 QUANTITATIVE ASSESSMENT OF THE REFERENCE DISPOSAL SYSTEM

The results of the quantitative assessment of the reference disposal system are discussed in the following seven related topics. The first five pertain to the analysis of the SYVAC scenarios and deal with derived constraints, median-value (deterministic) analysis, barrier effectiveness, probabilistic analysis, and a special study of assumed site and design features. The sixth and seventh topics describe the analyses for the open-borehole and inadvertent human intrusion scenarios.

Development of Derived Constraints

We use preliminary analyses to examine ways of improving the performance of the reference disposal system. Such analyses are considered preliminary because they can lead to a modification of the reference disposal system and to the associated models and data used in subsequent analyses.

For the studies described in this report, the constraint found to be most effective in reducing estimated annual doses involves a modification to the location and layout of the reference disposal vault. We then applied this modification and changed the original vault design. This design change is referred to as a derived constraint because it is determined by the system performance analysis.

The derived constraint involves a change to the vault layout relative to the nearby fracture zone LD1 (Figure ES-3). Fracture zone LD1 is a shallow-dipping fracture zone that we assume passes through the plane of the disposal vault, to connect at depth with a vertical joint. We also assume that LD1 sustains relatively high groundwater flow toward the surface. We observe the presence and assumed properties of LD1 have a strong influence on estimates of annual dose. (The properties of LD1 were based on information available in 1985, when a model of the hydrogeology of the WRA first became available. More recent information indicates that these assumptions represent an unduly pessimistic description of the groundwater flow system.) The derived constraint affects two aspects of the vault layout.

- The first involves the distance between LD1 and the vault. We assumed there would be a minimum of approximately 50 m of sparsely fractured rock between LD1 and the waste-emplacement part of any vault room. This distance is known as the waste exclusion distance (Figure ES-3).

- The second involves the orientation of vault rooms relative to LD1. We assumed that there would be no vault rooms containing nuclear fuel waste in positions above LD1. This is the situation shown in Figure ES-3, where all vault rooms are located below and to the left of LD1.

Figure ES-2 shows the modified vault design that is evaluated further in this document. In the original design, vault rooms were located above and below LD1, whereas in the modified design all the rooms are below LD1. The

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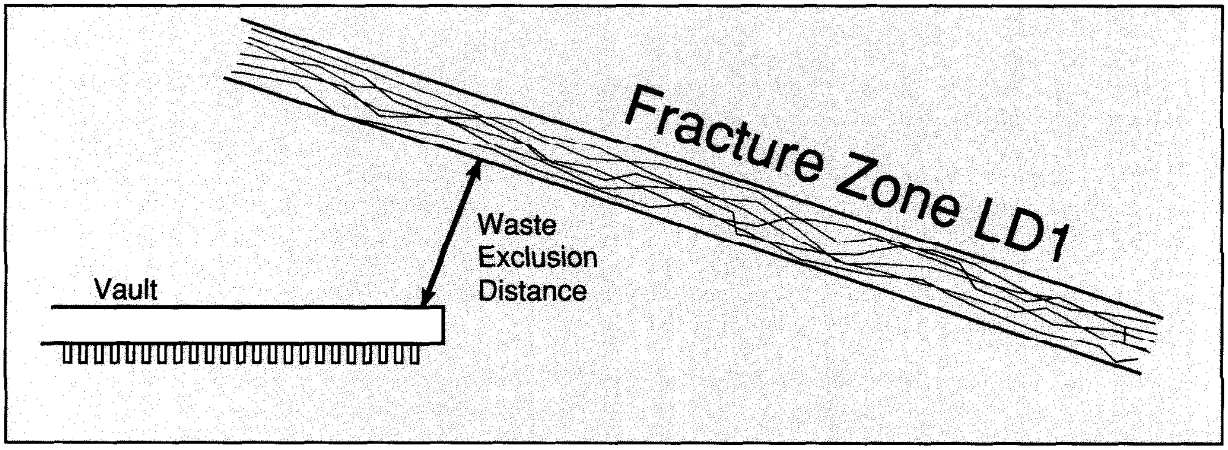

FIGURE ES-3: Orientation of the Vault Relative to Fracture Zone LD1

The final design for the reference disposal system assumes that no vault rooms are located above LD1, and that there is a distance of about 50 m (the waste exclusion distance) of sparsely fractured rock between any room containing nuclear waste and LD1.

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new design leads to several modifications to the reference disposal system and its system model. In particular, it changes the mass of used fuel in the reference disposal vault. In the conceptual design study (AECL 1994a, Simmons and Baumgartner 1994), the vault is about 2000 by 2000 m and contains 191 000 Mg U. For our analysis of the reference disposal system, we chose to eliminate the rooms above LD1 and to "remove" that part of the disposal vault within about 50 m of fracture zone LD1. That is, we reduced the dimensions of the disposal vault, such that its inventory of waste is about 15% smaller, or 162 000 Mg U.

One important qualification must be emphasized: this particular derived constraint is applicable only to the reference disposal system analyzed in this report.

<u>Summary of the Median-Value Results</u>

The deterministic analysis of the reference disposal system is based on a single simulation in which every parameter uses the median value of its PDF. We use this median-value simulation to study in detail the movement of contaminants through the vault, geosphere and biosphere, and to identify the principal pathways and factors affecting contaminant movement.

Figure ES-4 shows the estimated total annual dose and the most important contributors to the dose. The estimated total annual dose slowly increases to a value of 3 x 10^{-18} Sv/a at 10^4 a. For times up to 10^5 a, the estimated maximum in the total annual dose is 4 x 10^{-7} Sv/a. These estimates are far smaller than annual doses from radiation in the natural environment (about 3 x 10^{-3} Sv/a). Of the 68 radionuclides studied, most of the estimated annual dose is attributed to ^{129}I, with much smaller contributions from ^{14}C. Other radionuclides make far smaller contributions for times up to 10^5 a. Our analysis indicates there would be no significant releases into the biosphere of radionuclides such as cesium-135, strontium-90, tritium, technetium-99, uranium-235 and all isotopes of plutonium, americium and the other transuranics.

The analysis shows that the largest estimated annual doses are associated with one important flow path (Figure ES-5) in which contaminants move, principally by diffusion, from the waste forms, containers, buffer and backfill into the surrounding rock, and through the sparsely fractured rock to fracture zone LD1. When they reach fracture zone LD1, contaminants are transported by diffusion and by advection in moving groundwater to the intersection of LD1 and the well used by the critical group. Members of the critical group are mainly affected by eating food and drinking water that have been contaminated by water from the well, where the well is used as their source of domestic water, irrigation water and animals' drinking water.

We observe that radionuclides from only the three sectors of the vault closest to fracture zone LD1 contribute significantly to estimates of annual dose. These three sectors have a waste exclusion distance of about 50 m, whereas all other sectors are much farther from LD1, and thus make no consequential contribution to estimated doses for times up to 10^5 a.

Other results from the median-value simulation include estimates of where contaminants move in the reference disposal system. For example, by 10^4 a, about 3.9% of the total inventory of ^{129}I has left the waste containers and entered the buffer and backfill, and an extremely small fraction has reached the biosphere. For times up to 10^5 a, the estimated maximum entry rate of ^{129}I into the biosphere is about 1 x 10^{-5} mol/a from all pathways. Figure ES-6 illustrates these results.

Of the nine chemically toxic contaminants from the disposal vault, bromine has the greatest estimated discharge into the biosphere. The total discharge of bromine for times up to 10^5 a is about 0.11 mol, with a maximum estimated discharge rate of about 1 x 10^{-6} mol/a. The estimated concentration of bromine in the soil of the biosphere is less than 3 x 10^{-10} mol/kg, more than 5 orders of magnitude smaller than median concentrations of naturally occurring bromine in the environment. Similar observations apply to estimated concentrations of bromine in well water and in lake water. Discharge rates of the other eight chemically toxic contaminants are many orders of magnitude smaller than those for bromine, and estimated concentrations are far smaller than naturally occurring concentrations in the biosphere.

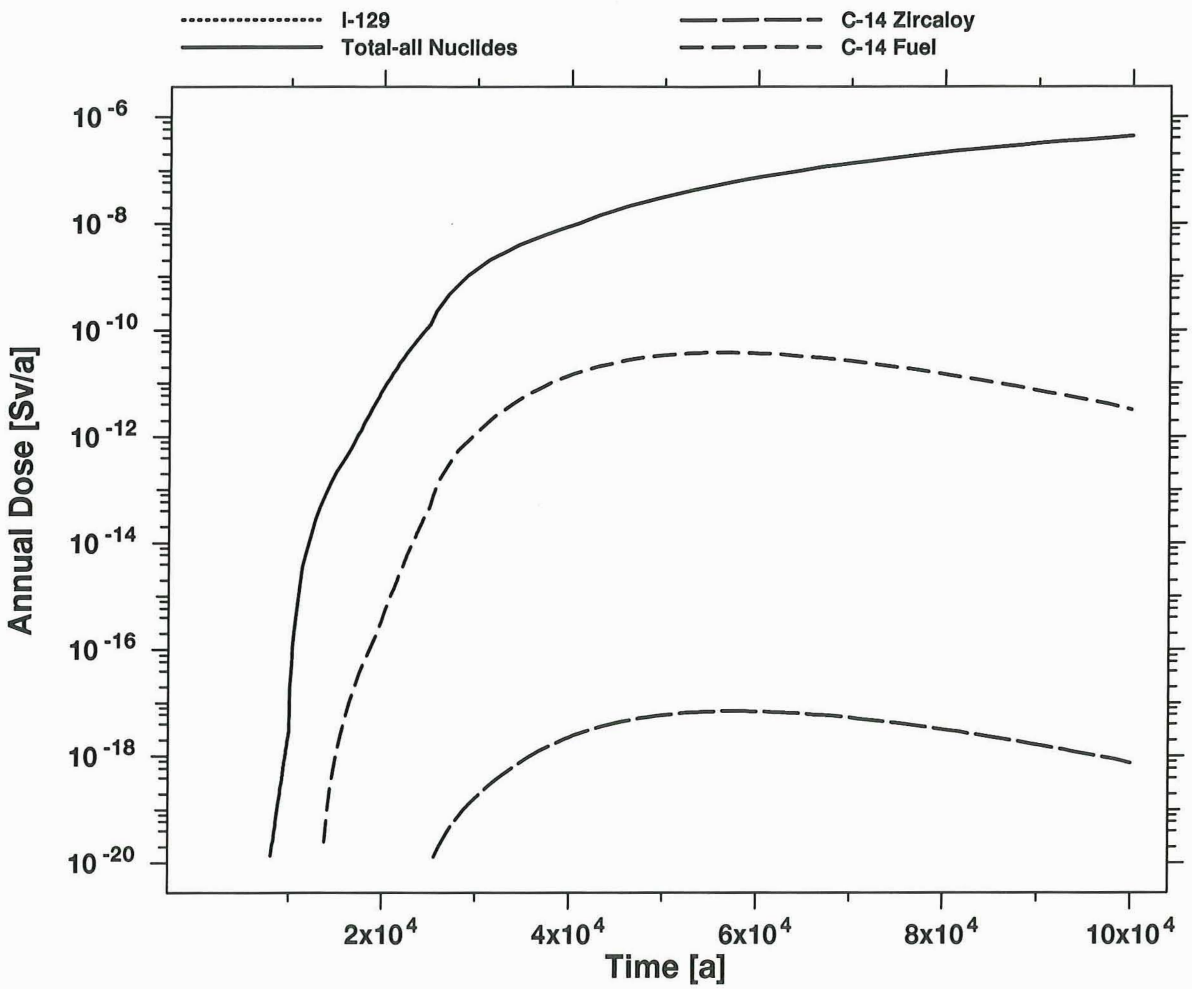

FIGURE ES-4: Estimated Annual Dose from the Median-Value Simulation

The major contributor to total estimated annual dose is ^{129}I: note that the total dose curve and the ^{129}I dose curve are identical in this plot. Estimated annual doses from ^{14}C (in both the used fuel and the Zircaloy sheaths), are orders of magnitude below the annual dose associated with the AECB risk criterion. Estimated annual doses from all other radionuclides are much smaller.

Estimated concentrations of all contaminants in the vicinity of the reference disposal vault are extremely small, even in those parts of the biosphere likely to be most contaminated. Subsequent effects on the environment are expected to be insignificant. In particular, estimated annual doses to nonhuman biota are much smaller than the total annual dose to plants and animals from natural sources.

Sensitivity analyses of the median-value simulation have identified the parameters that have the greatest influence on estimates of annual dose when their values are varied from their median values. As might be

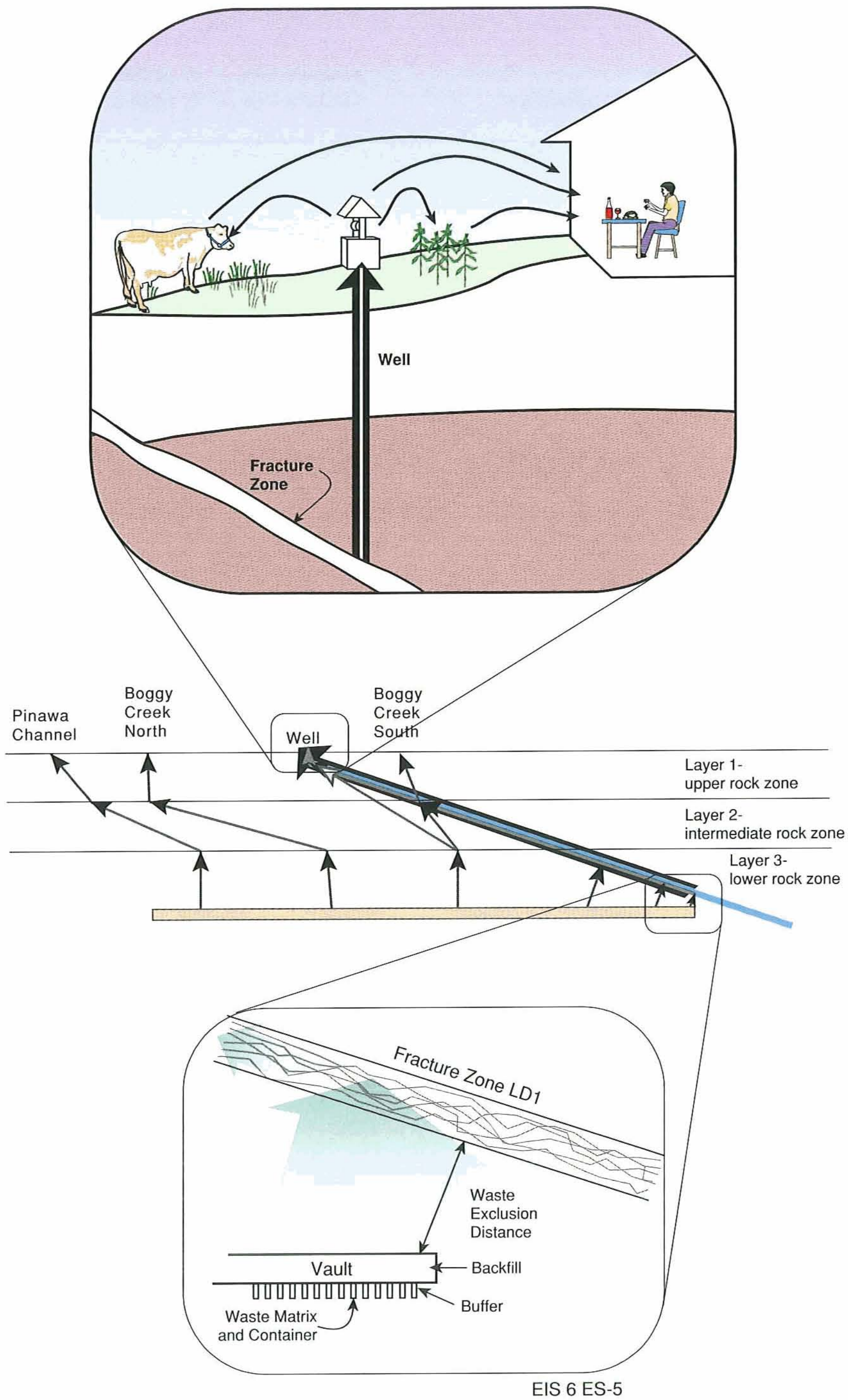

FIGURE ES-5: Principal Flow Path in the Median-Value Simulation

The main exposure pathway leading to the critical group starts from the vault sectors nearest fracture zone LD1 and includes transport upwards along LD1 to its intersection with the well.

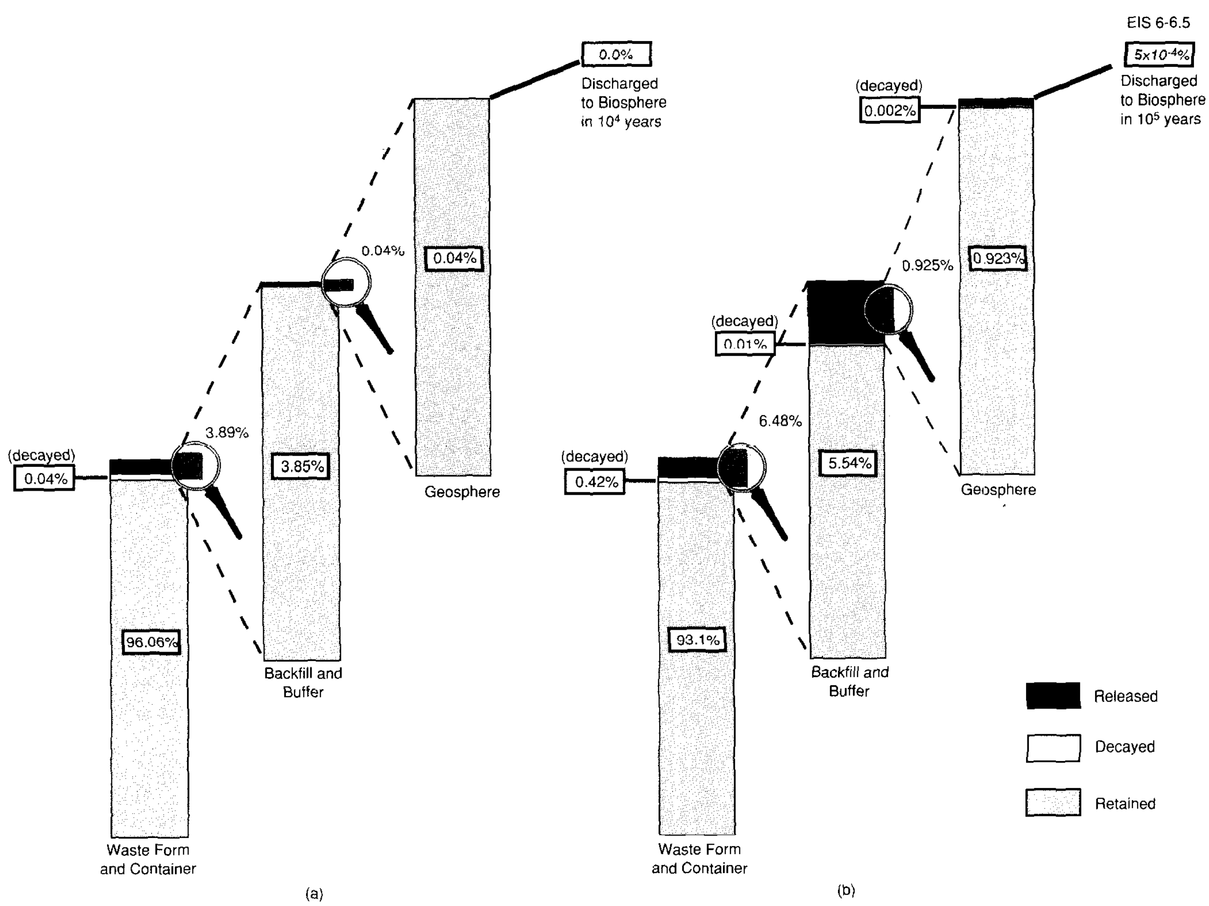

FIGURE ES-6: Distribution of ^{129}I in the Disposal System for the Median-Value Simulation

Parts (a) and (b) show the predicted distributions after 10^4 and 10^5 a respectively, expressed as percentages of the initial inventory of ^{129}I. Very small quantities of ^{129}I are released to the biosphere for times up to 10^5 a.

expected, many of these parameters relate to ^{129}I. For all such parameters, we have performed detailed studies to examine the underlying reasons for their importance.

Analysis of Barrier Effectiveness

The reference disposal system contains a number of engineered and natural barriers. A special sensitivity analysis is focussed on the relative effectiveness of eight barriers in the reference disposal system: the waste matrices (the used-fuel pellets and Zircaloy fuel sheaths containing the contaminants), the titanium containers, the low-permeability buffer surrounding the containers, precipitation of sparingly soluble elements in the buffer, the clay and crushed rock used as backfill for the rooms and tunnels in the vault, the rock within the waste exclusion distance, and the upper and lower portions of fracture zone LD1.

The analysis shows that the effectiveness of a barrier is a function of time and the properties of the contaminants. It concludes that most barriers are effective for most contaminants and that the combined effect of these multiple barriers leads to extremely small discharges to the biosphere for all contaminants (Figure ES-7). The analysis also shows that

- the most effective barriers are the used fuel and Zircaloy waste matrices, the backfill, the buffer, and the rock within the waste exclusion distance;
- there are only a few contaminants, notably ^{129}I and ^{14}C, for which several of the barriers are not effective; and
- every radionuclide is affected by several barriers.

This last observation applies even for ^{129}I and ^{14}C, the two radionuclides that dominate estimates of dose. For example, ^{129}I is affected by three independent barriers that offer approximately equal protection to 10^5 a: the waste matrices, the backfill and the rock within the waste exclusion distance.

Summary of the Probabilistic Results

The probabilistic analysis of the reference disposal system is based on thousands of simulations in which values for the model parameters are randomly sampled. That is, in each simulation, a value is selected for every parameter through random sampling of its associated PDF. The analysis examines

- Results from more than 40 000 simulations involving seven radionuclides expected to cause the largest annual doses (^{14}C, ^{135}Cs, ^{129}I, ^{59}Ni, ^{107}Pd, ^{79}Se and ^{99}Tc). Subsequent analyses confirmed that the only major contributors to estimated annual dose are ^{129}I and ^{14}C.

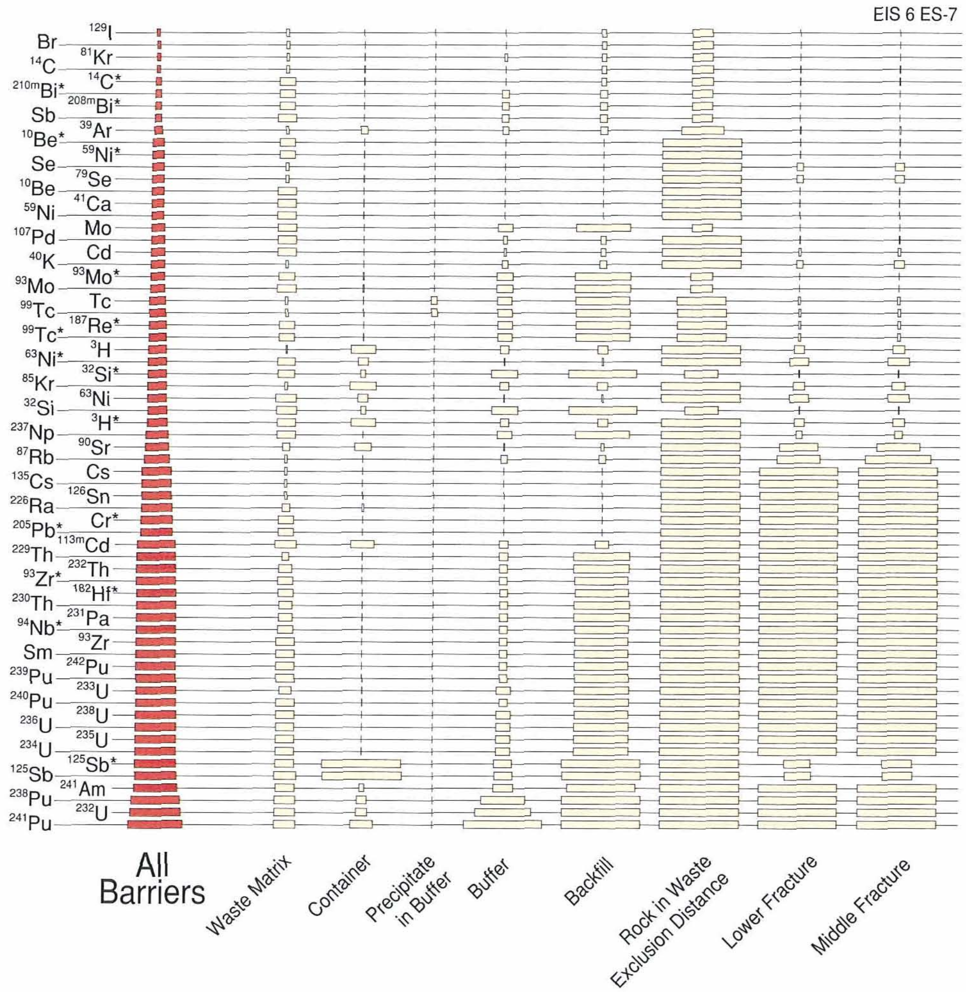

FIGURE ES-7: Summary of Barrier Performance at 10^4 a

This figure illustrates the relative effectiveness of eight barriers at 10^4 a after closure of the disposal vault. The labels on the left-hand side of the figure identify different contaminants ("*" indicates a contaminant from Zircaloy; all others are from used fuel). The first column of boxes represents a pessimistic value for the net effectiveness of a sequential combination of the barriers. The columns on the right indicate the relative effectiveness of the eight barriers, each considered individually. A longer box corresponds to a more effective barrier. The longest possible box (such as the five on the right for ^{241}Pu) means that essentially no contaminant passes through that barrier in 10^4 a. Calculation of these lengths involves a logarithmic transformation.

- Results from at least 2000 simulations for another 61 radionuclides and nine chemically toxic elements of concern for their potential impacts.

As noted earlier, we use the arithmetic average (or mean) of the estimated impacts from the large set of simulations for comparison with regulatory criteria. This average takes into account the effects of uncertainty in the values of the parameters. The results from the probabilistic analysis of the reference disposal system are as follows.

Radiological Impacts. The mean annual dose estimate to a member of the critical group slowly rises to a maximum of about 8 x 10^{-12} Sv/a for times up to 10^4 a (Figure ES-8). This value is far below the annual dose level of 5 x 10^{-5} Sv/a associated with the AECB risk limit (AECB 1987a). For times up to 10^5 a, the mean annual dose estimate rises to a maximum of about 1.3 x 10^{-6} Sv/a.

For all times up to 10^5 a, the mean annual dose estimate is clearly dominated by contributions from ^{129}I from used fuel (Figure ES-8). The second largest contributor is ^{14}C, and contributions from all other radionuclides are orders of magnitude smaller. (Recent data for ^{14}C suggest that we have significantly overestimated its contribution to the mean annual dose.)

The corresponding results from the median-value simulation are considerably smaller (estimated annual doses are 3 x 10^{-18} and 4 x 10^{-7} Sv/a for times up to 10^4 and 10^5 a respectively). Uncertainties associated with the reference disposal system lead to a distribution of estimated impacts that is highly skewed, such that the arithmetic mean dose is significantly greater than the corresponding single-dose estimate from the median-value simulation.

Chemical Toxicity Impacts. Estimated concentrations of all chemically toxic contaminants from the disposal vault in all parts of the local habitat of the critical group are so small that they would have negligible adverse impacts. For example, of the nine chemically toxic contaminants, bromine has by far the largest estimated concentrations in the biosphere. The mean of its maximum estimated concentration (up to 10^5 a) in soil is only 3 x 10^{-9} mol/kg, more than 10^5 times smaller than naturally occurring concentrations of bromine in typical soils. Mean concentrations of other contaminants are extremely small; most estimates are less than 10^{-20} mol/kg of soil and 10^{-20} mol/m^3 of water or air.

Protection of the Environment. Estimated concentrations of all radionuclides and chemically toxic elements in the most contaminated soil and water are compared with environmental baseline data. The results indicate that only two contaminants, ^{129}I and ^{14}C, could produce increases in their concentrations for the reference disposal system that are significant when compared with variations in their typical concentrations now found on the Canadian Shield. We have evaluated the potential effects of these two radionuclides. In particular, we estimate the radiation dose they could cause to four generic organisms (a bird, a mammal, a fish and a plant). These estimated annual doses are sufficiently small compared with the lower range of background radiation doses that potential radiological impacts would be negligible. Other impacts attributed to ^{129}I and ^{14}C are also negligible. We conclude that estimated concentrations

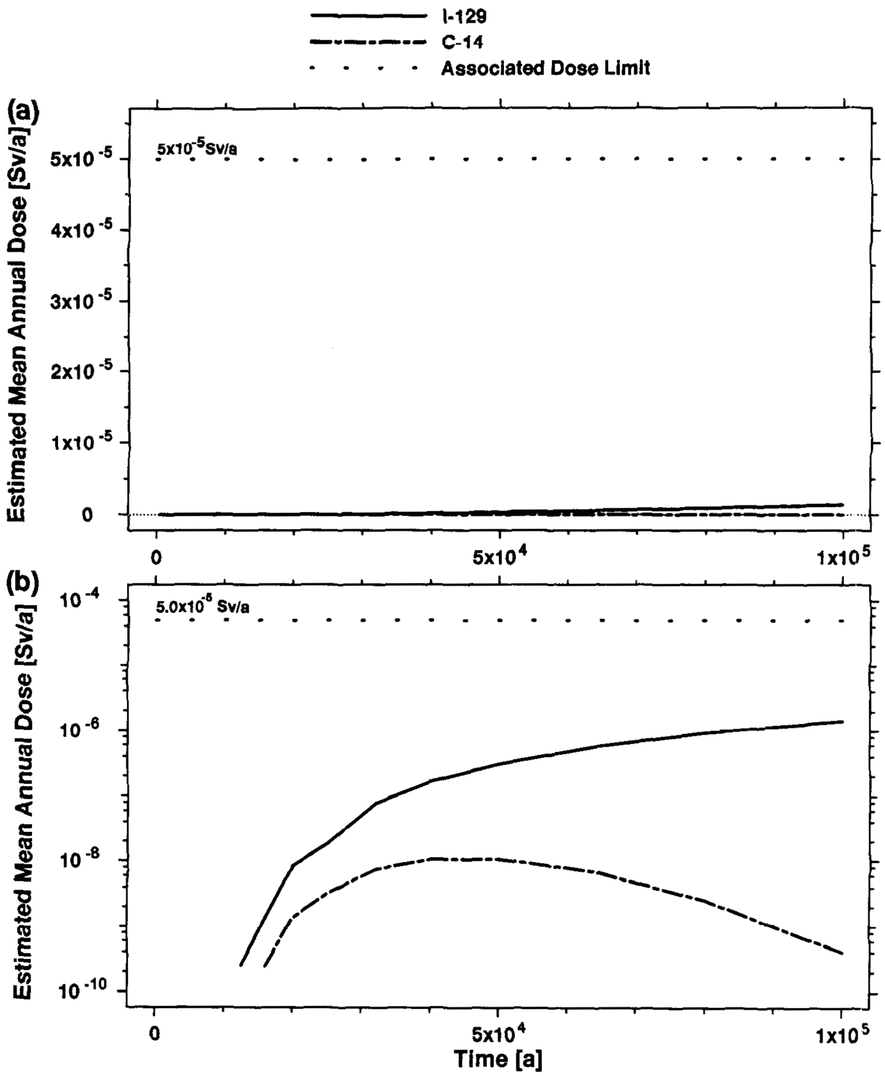

FIGURE ES-8: Estimated Mean Annual Dose from 40 000 Simulations

The curves show the arithmetic average (mean) of annual dose estimates from 40 000 simulations. The vertical axis is represented on both a linear (a) and logarithmic (b) scale. The dashed horizontal line shows the annual dose of 5 x 10^{-5} Sv/a associated with the AECB radiological risk criterion (AECB 1987a).

Iodine-129 is the dominant contributor, and its curve is indistinguishable from the total dose curve. Only one other radionuclide, ^{14}C, makes a significant contribution to the total.

> in the biosphere of all contaminants arising from the reference disposal vault are so small that no significant radiological or nonradiological impacts are expected.

The sensitivity analyses of the probabilistic results first screens the model parameters to identify those parameters that most influence the estimates of maximum annual dose (to 10^5 a), when considering the full ranges of possible values for all sampled parameters. Because this method of analysis can identify as important only those parameters that are characterized using PDFs, it cannot identify the waste exclusion distance as an important parameter because its value is fixed at about 50 m. However, we have identified these other important but fixed parameters using sensitivity analyses of the median-value simulation. (We have also studied their effects; for instance, the effects of varying the waste exclusion distance are included in the special studies described in the next section.)

Eight parameters were found to be most important: the tortuosity of the lower rock zone, the groundwater velocity scaling factor, the retardation factor of iodine in compacted organic lake sediment and the thickness of the sediment, the free-water diffusion coefficient for iodine, the buffer anion correlation parameter, the switch parameter determining whether domestic water comes from the well or the lake, and the depth of the well. Of these, the two most important are related to the characteristics of the sparsely fractured rock surrounding the vault, including the rock within the waste exclusion distance. They are the tortuosity of the lower rock zone and the groundwater velocity scaling factor. The first parameter is a measure of the increase in the effective distance for transport by diffusion arising from the winding nature of the interconnected aqueous pathway. The second is a measure of the uncertainty associated with groundwater velocities in the geosphere. Another important parameter determines whether the well or the lake serves as the source of drinking water used by members of the critical group. All eight parameters influence the movement of ^{129}I from the disposal vault to the critical group.

The effects of these eight important parameters have been examined in detail. For example, we show that larger estimates of annual dose are generally associated with smaller values of tortuosity, with larger values of the groundwater velocity scaling factor, and with the well serving as the source of drinking water. In addition, we identify, and then examine the influence of many other parameters that are important because of their effects in the vault, geosphere and biosphere models.

Several tests confirm that we have identified the parameters whose uncertainties cause nearly all the variability in the maximum dose estimates to 10^5 a. These parameters, therefore, would be primary candidates for further study to determine their possible values more accurately. A special analysis of the tortuosity of the lower rock zone examines how more information for this most important parameter could affect the magnitude and variability of the estimated mean annual dose for the reference disposal system.

Effects of Assumed Site and Design Features

Special sensitivity analyses of the probabilistic results are used to examine the effects of assumed site and design features. The studies are "special" because they examine ranges of parameter values that are beyond the values specified for the reference disposal system. Thus the results must be examined with caution. However, they do provide more information on the reference disposal system, and illustrate how a postclosure assessment can contribute to the evaluation of different features and different ways to improve the performance and safety margin of an actual disposal system. The studies are similar to those described at the beginning of Section ES.3, except that they take into account the effects of parameter uncertainty and variability.

Assumed features that are examined include more durable containers, thicker layers of buffer and backfill, different waste exclusion distances, placement of vault rooms in a hydraulically favoured location, smaller groundwater velocities, larger concentrations of naturally occurring stable iodine in the groundwater, larger watershed areas, and wells used by members of the critical group that do not intersect the plume of contaminants. Figure ES-9 shows the results and indicates that three design constraints would be most effective in reducing the mean annual dose estimates for times up to 10^5 a: locate vault rooms only below LD1 (that is, eliminate any vault rooms located above LD1), increase the waste exclusion distance, and use very durable (long-lived) containers. (In the development of derived constraints discussed at the start of Section ES.3, we used the first two of these constraints to modify the original design of the vault. The analysis here indicates these same constraints would still be very effective.)

Evaluation of the Open-Borehole Scenarios

The open-borehole scenarios describe a situation in which one or more open boreholes could allow contaminants to by-pass a large fraction of the geosphere barrier, and thus provide a potentially significant transport pathway for contaminants in the disposal vault (Figure ES-10). Boreholes would be drilled during all stages of the project, but typically only about 20 deep exploration boreholes would be drilled from the surface and near the potential area of a disposal vault for site characterization.

From our evaluation for the reference disposal system, we conclude that the potential for open-boreholes would not make a significant contribution to the radiological risk if three quality assurance procedures were used during the project to minimize the likelihood that a borehole would remain open at the time of vault closure.

1. Ensure that all boreholes are properly sealed when no longer needed, following a quality assurance procedure that would be in effect during all stages of the disposal project.

2. Avoid during the construction stage locating any vault room containing nuclear waste within some minimum acceptable distance of any deep exploration borehole.

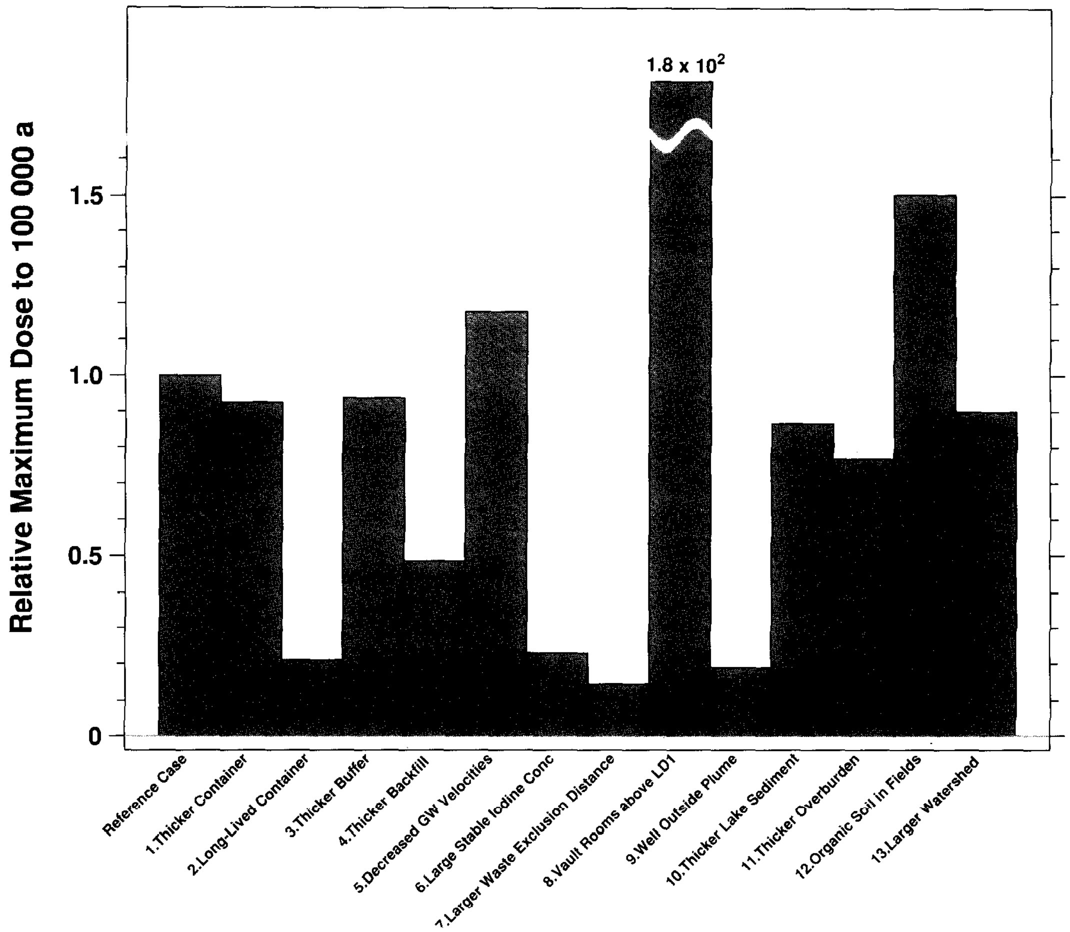

FIGURE ES-9: Effects of Assumed Site and Design Features

Effects of different assumed site or design features are shown relative to the reference case. The comparisons use the means of the maximum estimated doses, to 10^5 a, from 500 randomly sampled simulations.

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3. Confirm using geophysical detection methods prior to closure that there are no open boreholes near any vault rooms containing nuclear fuel waste.

A borehole would remain open at the time of vault closure only if there was a failure to seal the borehole, a failure to isolate vault rooms containing waste from all deep boreholes by some minimum distance, and a failure to detect the presence of the borehole near a vault room. We believe that quality assurance procedures would provide a sufficiently high degree of confidence that no boreholes would remain open at the time of vault closure

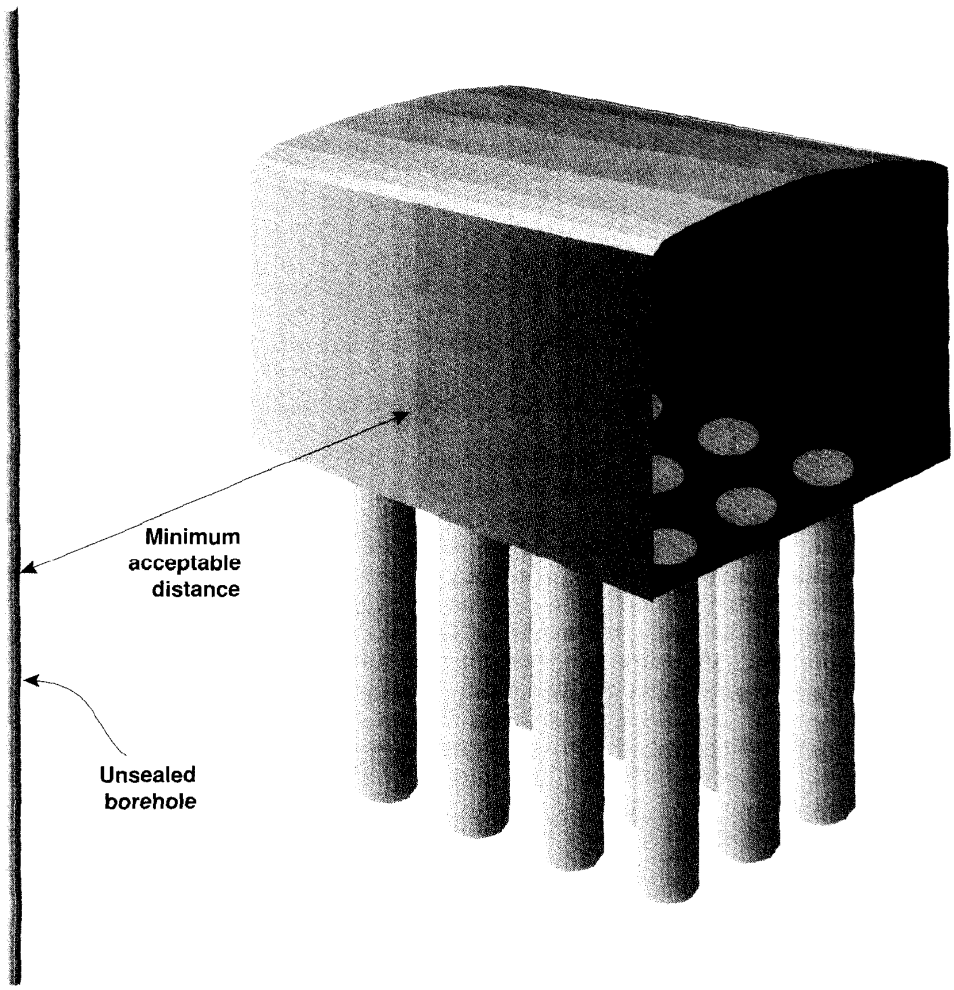

FIGURE ES-10: Feature of Interest for the Open-Borehole Scenarios

These scenarios deal with an open borehole that passes near the vault and extends upwards to the surface. Our analysis indicates that the open-borehole scenarios would not contribute significantly to the radiological risk because of the application of three redundant quality assurance procedures that would ensure all boreholes are properly sealed, isolate vault rooms containing nuclear fuel waste from any deep boreholes by some minimum acceptable distance, and confirm there are no open boreholes near any vault room.

that would affect the performance of the disposal system. Thus the open-borehole scenarios would not contribute significantly to the radiological risk.

Our evaluation of the open-borehole scenarios includes quantitative analysis of results from SYVAC3-CC3. This analysis indicates that, for the reference disposal system, a minimum acceptable distance of an open borehole to a vault room containing waste is likely to be less than 30 m. That is, if an open borehole were about 30 m distant from any room containing nuclear fuel waste, it would not contribute significantly to the radiological risk. Another analysis, using a modified version of SYVAC3-CC3, provides a representative estimate of the effects of an open borehole for the reference disposal system. These latter results suggest that an open borehole would not produce a large annual dose, even if it passed as close as about 5 m from a vault room containing nuclear fuel waste.

Evaluation of the Inadvertent Human Intrusion Scenarios

The inadvertent human intrusion scenarios describes radiation exposures caused by human actions at the disposal site after the closure of the disposal facility. We assume that these actions are unintentional, or inadvertent, in the sense that they are carried out without knowledge of the presence of a disposal vault and its potential hazards. We examine the effects of actions initiated by a low-probability drilling operation that leads to the direct removal of nuclear waste from the disposal vault to the surface environment, thereby by-passing all natural and engineered barriers. (Some more probable future human intrusion actions are included in the SYVAC scenarios, such as drilling a water-supply well into the rock at the disposal site and farming on land or lake sediment located at the discharge areas of groundwater that has passed through the vault.)

We estimate the probabilities of occurrence and annual doses for four related scenarios in which different individuals are most at risk. Two scenarios deal with exposure to the undispersed waste brought to the surface, and the individuals most at risk are a member of the drilling crew and a laboratory technician. The other two scenarios deal with exposure to waste that has been dispersed over some site on the surface, and the individuals most at risk are a construction worker and a resident of a house at the site.

The probabilities of occurrence of these scenarios change with time for reasons such as the assumed loss of effectiveness of active and passive institutional controls. However, the estimated probabilities of occurrence are very small just after closure of the disposal vault, and are less than 5×10^{-6} for all times up to 10^4 a. In contrast, estimated annual doses are largest at earlier times when the waste is most radioactive, but decrease at longer times.

The radiological risk is calculated using the risk equation specified by the AECB (1987a), modified to account for acute annual doses larger than 1 Sv/a. The largest calculated risks are associated with the drill-crew and resident scenarios and both reach peak values of about 3×10^{-10} serious health effects per year (Figure ES-11). These peak values occur

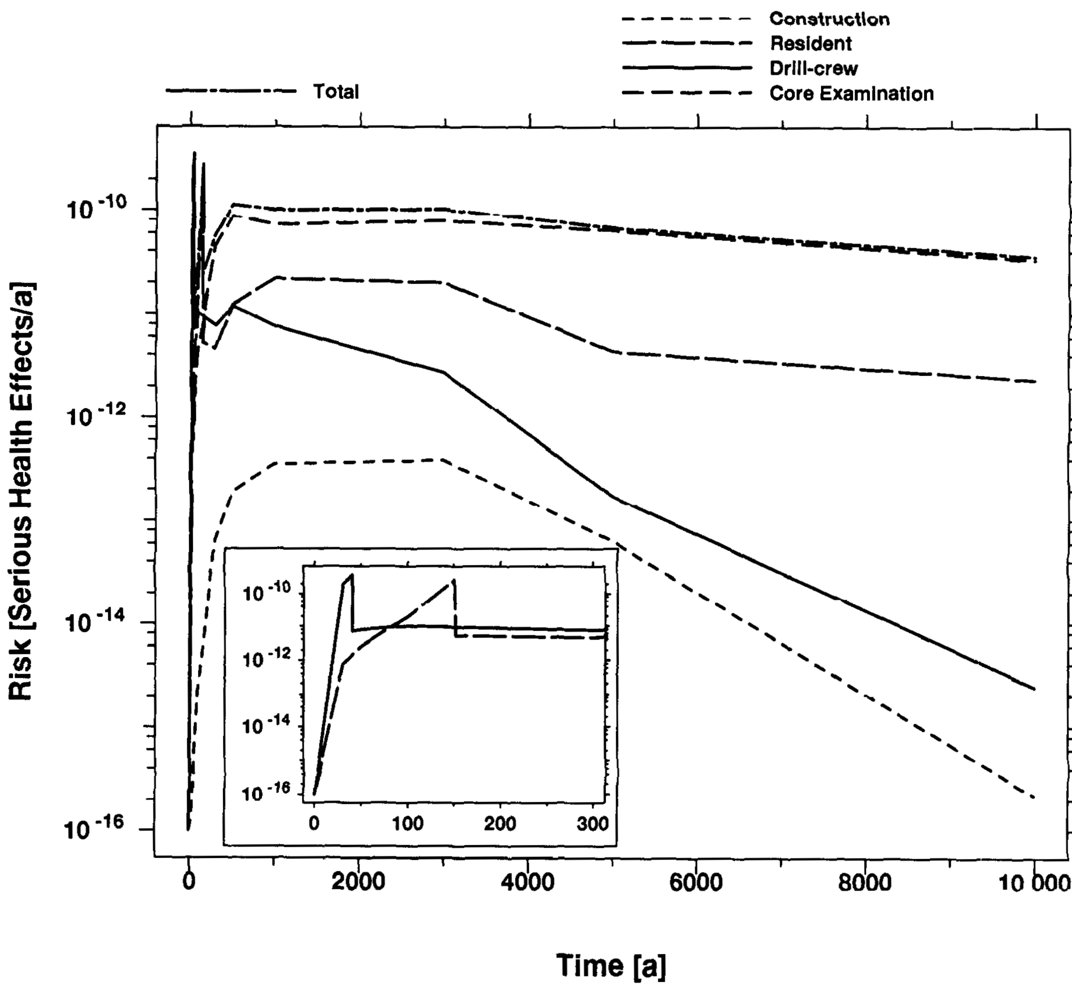

FIGURE ES-11: Estimated Risk from Inadvertent Human Intrusion

The four lower curves show the calculated radiological risk for the drill-crew, core examination, construction and resident scenarios; they are summed in the upper "total" curve. The maximum for each curve is at least 3000 times smaller than the risk criterion (AECB 1987a). The inset shows a blowup for times up to 300 a, and for the drill-crew and resident scenarios. These curves show discontinuities near 40 a and 150 a, the consequence of a modification to the risk equation.

near 40 a and 150 a respectively. Smaller risks are associated with the core-examination and construction scenarios.

If we assume the same individual is the member of the drilling crew, the laboratory technician, the construction worker and the resident, the radiological risk would reach peak values of about 3 x 10^{-10} serious health effects per year. The calculations also show that the radiological risks slowly decline after about 500 to 3000 a, and continue to decline at 10^4 a, because estimated annual doses are decreasing faster than estimated probabilities of occurrence are increasing. We conclude that the risk associated with the inadvertent human intrusion scenarios are about 3000 times smaller than the AECB risk criterion (AECB 1987a).

ES.4 LONG-TERM IMPACTS OF THE DISPOSAL SYSTEM

The AECB regulations (AECB 1987a) require that, if estimates of annual dose to members of the critical group do not reach a maximum within the first 10^4 a following closure, reasoned arguments must be presented to show that radionuclide releases to the environment will not suddenly and dramatically increase, acute radiological risks will not be encountered by individuals, and major impacts will not be imposed on the biosphere.

Because our results for the SYVAC scenarios show that the estimated annual dose continues to rise past 10^4 a, we have extended the analysis to much longer times. The discussion in this report is focussed on potential long-term impacts for an undisturbed reference disposal system, taking into consideration quantitative results from the SYVAC scenarios for times up to 10^5 a, supplemented with reasoned arguments to cover longer time-scales. The EIS (AECL 1994a) provides more general discussions on potential effects of disruptions and disturbances that could occur over long time frames, such as glaciation, earthquakes, meteorite impact and human intrusion.

Impacts for an Undisturbed Disposal System

From our analysis of the undisturbed reference disposal system using SYVAC3-CC3, we observe that

- For times up to 10^5 a, the estimated annual dose is much smaller than the annual dose associated with the AECB risk criterion, and even further below the total annual dose from naturally occurring sources of radiation.

- Carbon-14 and ^{129}I are the only radionuclides released to the environment in any appreciable quantities for times up to 10^5 a. Carbon-14 and ^{129}I have four characteristics that lead to this important observation: they are relatively long-lived, a significant fraction of their inventories is available for release from the used-fuel waste matrix at the instant of water ingress, they are relatively abundant in used fuel, and they are relatively mobile both in the vault and in the rock surrounding the vault. No other radionuclide has all these characteristics.

Thus other radionuclides with nonzero instant-release fractions do not make significant contributions to dose. (They are ^{39}Ar, ^{135}Cs, ^{3}H, ^{81}Kr, ^{85}Kr, ^{40}K, ^{87}Rb, ^{79}Se, ^{90}Sr, ^{99}Tc, and ^{126}Sn.)

- There are no significant contributions to total dose for times up to 10^5 a from the inventory of any radionuclide that is released congruently with the dissolution of the used-fuel and Zircaloy matrices. Both of these matrices are expected to persist, relatively unchanged, for very long times under the geochemical conditions of the disposal vault. Radionuclides such as ^{237}Np, ^{239}Pu, ^{241}Am, ^{226}Ra and ^{235}U are contained within the used-fuel waste matrix, and are released only when the matrix dissolves through the "congruent" release mechanism.

- The maximum in the mean annual dose estimate for ^{14}C occurs before 10^5 a, and this maximum is far smaller than the annual dose associated with the AECB criterion. The mean annual dose estimate for ^{129}I is still rising at 10^5 a. However, internal doses from ^{129}I cannot normally lead to an acute risk to a member of the critical group because of the way that ^{129}I behaves in the human body.

- Radionuclides with half-lives shorter than that of ^{14}C (5×10^3 a) will decrease in inventory by a factor of more than a million after 10^5 a. Because these radionuclides have not made a significant contribution to dose by 10^5 a, their contributions for times after 10^5 a would be negligible. (This point does not apply to a small number of progeny radionuclides whose inventories might increase substantially in time because of ingrowth.)

Over time frames of millions of years, the vault inventory would be largely dominated by uranium and its decay products. At these long times, the waste vault resembles a high-grade uranium ore deposit, the behaviour of which provides a natural analogue to the performance of the vault and the radionuclides it would contain.

Our studies of the Cigar Lake ore deposit in Northern Saskatchewan have focussed on particular aspects that have parallels with our reference disposal system. These studies indicate that the ore is thermodynamically stable in the geochemical environment of the ore deposit, has remained in place for millions of years, has undergone extremely slow congruent dissolution, and has retained most of its nuclear reaction products (Cramer 1994). An important reason for these observations is connected with the geochemical environment found at the Cigar Lake deposits: the uranium ore is located in a reducing electrochemical environment and is surrounded by several naturally occurring barriers such as a layer of clay. We expect an electrochemical environment in the disposal vault and surrounding geosphere that would be reducing and that would persist for millions of years in an undisturbed disposal system. We also expect the low-permeability clay buffer would remain in place for times far beyond 10^5 a.

It is reasonable to expect that long-term environmental impacts attributed to the undisturbed reference disposal vault would lie somewhere in the range of environmental effects observed today from deeply buried naturally occurring uranium ore deposits. Studies of potential health hazards from nuclear fuel waste and from uranium ore deposits show they have about the same level of hazard for times beyond about 10^4 a (Mehta 1988, Mehta et al. 1991).

From the above considerations for the undisturbed reference disposal system, we expect that major impacts would not be imposed on the biosphere, that any radionuclide releases would be gradual (rather than sudden and dramatic), and that annual doses would be of the level now present in nature and far below levels associated with acute doses or acute radiological risks.

The EIS (AECL 1994a) presents further discussion on the potential effects of disturbances and disruptions to the disposal system.

ES.5 SUMMARY AND CONCLUSIONS

We draw the following conclusions from our analysis.

Three types of scenarios are evaluated for the reference disposal system: the SYVAC, open-borehole and inadvertent human intrusion scenarios. We have estimated their probabilities of occurrence and their potential impacts.

- We show that calculated radiological risks are much smaller than the the AECB radiological risk criterion for all times up to 10^4 a. For the SYVAC scenarios, the calculated risk reaches a maximum value of about 2×10^{-13} (chances of receiving a serious health effect per year) at 10^4 a following closure of the disposal vault. The open-borehole scenarios would not contribute significantly to the radiological risk if quality assurance procedures are administered effectively during the project. For the inadvertent human intrusion scenarios, the calculated risk reaches a maximum value of about 3×10^{-10} within about 300 a following closure. The total risk, therefore, is at least 3000 times smaller than the the AECB risk criterion for all times up to 10^4 a.

- We show that the reference disposal system would meet regulations and guidelines pertaining to chemically toxic contaminants. Estimated concentrations of chemically toxic contaminants are many orders of magnitude smaller than naturally occurring concentrations in the environment and would have no significant effect on members of the critical group.

- We show that the reference disposal system will meet guidelines for protection of the environment. Only ^{129}I and ^{14}C exceed environmental baseline data; however, their chemical toxicity and radiotoxicity effects would be negligible. Specifically, estimated annual doses to four generic nonhuman organisms are far below the lower limit of total background dose rate.

- The safety offered by the reference disposal system will extend far into the future. An evaluation of impacts for longer time frames shows that rates of release of contaminants would not suddenly and dramatically increase, no acute radiological risks would be expected, and no major impacts would be imposed on the biosphere.

We have also identified design and engineering constraints that would improve the margin of safety of the reference disposal system, and it has identified components of the system that have the strongest influence on uncertainty in the estimates of impact.

The study results clearly support the conclusion that the reference disposal system would meet the relevant requirements for public safety and protection of the environment. In addition, if the assessment pertained to an actual candidate site, the results would support a decision to proceed with further exploratory studies, including exploratory excavation.

1. INTRODUCTION

1.1 BACKGROUND

1.1.1 Context of This Report

AECL Research and Ontario Hydro were assigned responsibility in 1978 for the Canadian Nuclear Fuel Waste Management Program (CNFWMP), to evaluate the concept for deep underground disposal of nuclear fuel waste in intrusive igneous rock of the Canadian Shield (Joint Statement 1978, 1981). The disposal concept is being reviewed by a federal Environmental Assessment and Review Panel (EARP), which has issued guidelines (EARP 1992) for the preparation of an Environmental Impact Statement (EIS). AECL is submitting the EIS (AECL 1994a,b) to the Panel, and the Panel will make it available for public and regulatory review.

This report is a primary reference to the EIS; that is, it provides detailed support for some of the material discussed in the EIS.

1.1.2 Scope of This Report

This report presents a long-term environmental and safety assessment, referred to hereafter as the postclosure assessment. It documents

- the approach that was developed to estimate and evaluate the long-term impacts of a disposal facility on human health and the natural environment, and

- an application of the approach to a hypothetical implementation of the concept.

The postclosure assessment examines the long-term performance and behaviour of the disposal system. It starts from the time the disposal facility is closed, that is, after all the shafts, tunnels and boreholes have been sealed, and it extends far into the future. Another primary reference, the preclosure assessment (Grondin et al. 1994), deals with the activities that precede and include the closure of the disposal facility.

The postclosure assessment applies to a hypothetical implementation of the concept, referred to in this document as the reference disposal system. Most of the analyses presented in this report pertain to the postclosure assessment of this reference disposal system.

One inherent qualification must be noted with regard to this assessment of the reference disposal system: it is equivalent to preliminary studies that would be conducted during the evaluation of a potential disposal site. If a decision were made to implement the disposal concept, then it is anticipated that implementation would proceed through several stages (AECL 1994a):

- siting (with site-screening and site evaluation substages), to identify a small number of sites for detailed investigation, and then to identify a preferred site and to obtain approval for construction at that site;

- construction, to fabricate the disposal facilities and to obtain approval to begin waste emplacement;
- operation, to emplace nuclear fuel waste in the disposal vault;
- extended monitoring, to obtain approval for starting the decommissioning of the disposal facility;
- decommissioning, to complete the sealing of the disposal vault and to rehabilitate the site;
- extended monitoring, to obtain approval to begin closure; and
- closure, to return the site to a passively safe state (or a state such that safety would not depend on institutional controls).

Postclosure assessments would contribute to the decision-making process at each stage:

- During the site-screening substage, postclosure assessments of potentially suitable sites would help to determine the technical merits of these sites, largely on the basis of information derived from reconnaissance studies. Results from the postclosure assessment would contribute to selecting a small number of areas for more detailed investigation.
- During the site evaluation substage, more detailed information would become available for each potential site, particularly from subsurface studies of the geosphere. Postclosure assessments using more detailed information would contribute to evaluating the technical acceptability of each potential site, to selecting a preferred site and to obtaining approvals for the construction stage at a preferred site.
- For the selected site, postclosure assessments would continue, incorporating the growing volume of detailed site-specific information that would be obtained during the construction, operation, decommissioning and extended monitoring stages. Results from postclosure assessments would play a role in each stage; for example, identifying design and operational constraints that would be effective and appropriate during construction. Results from the postclosure assessments would also contribute to the eventual decision to close the facility.

On the basis of information available for the reference disposal system, the application of the postclosure assessment described herein is approximately equivalent to interim investigations that would be conducted during the evaluation of one potential site. In particular, our assessment corresponds to what could be done at a time when there was substantial information from studies on the surface and in exploration boreholes, but when no exploratory excavation had been done. Thus it demonstrates how the postclosure assessment methodology could be used when deciding whether or not to begin exploratory excavation at a preferred disposal site.

1.1.3 Readers of This Report

The material in this document is technical in nature. The authors assume that the reader has a general knowledge of physics, chemistry, biology and mathematics. Condensed and less technical overviews of the postclosure assessment and results may be found in the

- *Environmental Impact Statement on the Concept for Disposal of Canada's Nuclear Fuel Waste* (AECL 1994a), and

- *Summary of the Environmental Impact Statement on the Concept for Disposal of Canada's Nuclear Fuel Waste* (AECL 1994b).

We have included extended captions with most of the figures, so that a reader might more quickly review different parts of the report by examining the figures. The main text accompanying each figure provides more details.

1.1.4 Organization of This Report

We have organized this report as follows:

- In the following sections of this chapter, we outline the general goals and scope of the postclosure assessment. We then describe the relevant regulatory requirements and indicate the manner of compliance for our assessment of the reference disposal system.

- Chapter 2 describes the method developed to estimate the postclosure impacts of the deep underground disposal of Canada's nuclear fuel waste. We describe its application for the reference disposal system in the remainder of the report.

- In the next three chapters, we describe three major activities that precede the evaluation of impacts. In Chapter 3, we describe the system to be evaluated; in Chapter 4, we identify the important features of the system; and in Chapter 5, we specify a system model and associated data required for the assessment.

- In Chapter 6, we discuss the quantitative results from the postclosure assessment of the reference disposal system. These results describe the estimated impacts for the first 10^4 a following closure of the hypothetical disposal facility.

- Chapter 7 presents reasoned arguments that examine estimated impacts from the reference disposal system for times beyond 10^4 a following closure. More general arguments are supplied in the EIS (AECL 1994a).

- In Chapter 8, we discuss the conclusions of the assessment. We also provide comments related to future assessments of a real disposal system.

The appendices provide more technical detail on the following special topics:

- Appendix A describes the tools used to prepare the quantitative estimates of impact for postclosure assessment.

- Appendix B gives information on the quality assurance measures that were applied to the development of computer models and software.

- Appendix C discusses three Atomic Energy Control Board (AECB) Regulatory Documents: R-71 (AECB 1985), R-104 (AECB 1987a) and R-72 (AECB 1987b), which contain important regulations, guidelines and criteria pertaining to the disposal of nuclear fuel waste.

- Appendices D to F present more details of the underlying analyses.

Additional information may be found in the references listed at the end of this document. Three references are especially important because they describe the underlying support for the models and data used in this postclosure assessment. They are the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993).

1.1.5 Other Postclosure Assessment Studies

A comparison with the waste management programs of other countries helps to put the concept for disposal of Canada's nuclear fuel waste assessment program into perspective. Of particular interest are the programs of Sweden (SKBF/KBS 1983, SKB 1992), Switzerland (NAGRA 1985), Germany (Storck 1989, Buhmann et al. 1991), the United States (Eslinger et al. 1989), Belgium (Bonne and Marivoet 1989) and the Commission of the European Communities (PAGIS 1988). Most of these programs have recently published assessments of deep geological disposal of nuclear fuel waste.

Among these programs, there are differences in the details of the approach to the development and assessment of a disposal concept. These differences include the choice of analytical methods and the performance and safety criteria, guidelines and standards. The exchange of ideas and critical reviews among the various assessment teams has contributed significantly to the quality of all their assessments, including the assessment work summarized in this report.

Other types of cooperation have also been valuable, such as the exchange of data, computer code comparisons, and cooperative experimental programs. Examples of the latter programs are those presently under way at the Underground Research Laboratory (URL) near the Whiteshell Laboratories (WL) in Canada and at the former iron mine in Stripa, Sweden. As well, international information exchange projects have been instituted in several technical fields, such as groundwater and radionuclide chemistry, the health effects of radionuclides, and the techniques of performance and safety assessment.

1.2 OBJECTIVES OF THE POSTCLOSURE ASSESSMENT

The principal objectives of the postclosure assessment case study are

1. to develop and document a method for estimating and evaluating the long-term effects and safety of a facility for the disposal of Canada's nuclear fuel waste; and

2. to demonstrate the utility of the method by applying it to the reference disposal system, a hypothetical implementation of the concept.

The method we have developed is based on a risk assessment methodology. The Canadian Standards Association (CSA) provides the following definitions:

> Risk assessment [is] the process of risk analysis and risk evaluation.
>
> Risk analysis [is] the use of available information to estimate the risk to individuals or populations . . . . Risk analysis is a structured process that attempts to identify both the extent and likelihood of consequences associated with [technological] hazards.
>
> Risk evaluation [is] the stage at which values and judgments enter the decision process, explicitly or implicitly, by including consideration of the importance of estimated risks . . . .
>
> Risk [is] a measure of the probability and severity of an adverse effect to health, property, or the environment. Risk is often estimated by the mathematical expectation of the consequence of an adverse effect occurring (i.e., the product of probability x consequence) (CSA 1991).

The CSA also notes that the "various life cycle phases" of risk analysis include the "Concept and Definition/Design and Development Phase" (CSA 1991). Our study of the reference disposal system has specific objectives corresponding to this phase (Figure 1-1):

- to identify possible long-term environmental and safety effects, notably the radiation dose to members of the critical group, and to estimate the magnitudes of the impacts;

- to compare the magnitudes of these effects with safety criteria, regulations and guidelines established by regulatory agencies in Canada, such as the radiological risk criterion set forth by the AECB (AECB 1987a); and

- to conduct sensitivity analyses to identify factors and derived constraints that could have an important influence on the estimated annual radiation dose to members of the critical group.

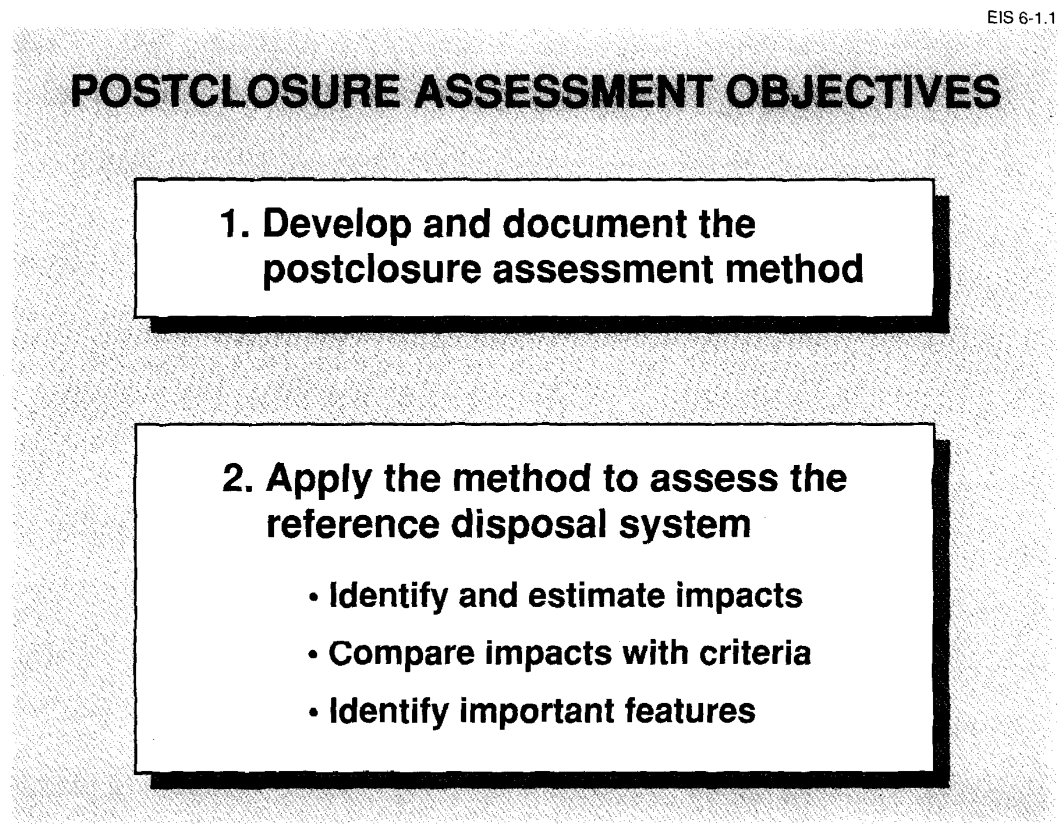

FIGURE 1-1: Objectives of the Postclosure Assessment

The first objective is to develop and document a method for estimating and evaluating the long-term effects and safety of a facility for the disposal of Canada's nuclear fuel waste. The second objective is to demonstrate the application of the method; we do so for an assessment of a hypothetical implementation of the concept, called the reference disposal system in this document. Specific objectives of the application are to identify and estimate possible impacts, including radiation and chemical toxicity effects; to compare these impacts with environmental safety criteria, regulations and guidelines; and to perform sensitivity analyses to identify important features of the system.

A factor is any feature, event, or process that could influence the performance of any component of the disposal system. Derived constraints include possible restrictions or modifications that, if applied to the reference disposal system, would increase the margin of safety. (Other derived constraints may contribute to the selection of a real disposal site and to the optimization of a real disposal system.)

In the following notes, we outline some key points that pertain to the definition of risk and how it is estimated. Further discussion is provided in Chapter 2 and Appendix C.

- There is no widespread agreement on the meaning and definition of risk, nor on the conversion of small dose rates to risk (see Wynne (1989), Garrick (1989) and Harris (1992)). Although the mathematical definition is unambiguous, the term "risk" has different connotations to different people. For example, Morgan (1993) notes that "risk space" includes human perceptions on the hazard's "dreadfulness" and how well the hazard is understood.

  Thus where possible, we provide in this assessment more fundamental end points or impacts, such as the radiation dose to the most exposed group of people and concentrations of contaminants in the soil, water and air in the local habitat of the critical group. (Contaminants include both radioactive and nonradioactive nuclides from the nuclear fuel waste.) This is the case for the high-probability scenarios. We also evaluate scenarios that have very small probabilities of occurrence and large estimates of radiation dose. For these low-probability large-consequence cases, it can be misleading to consider only the estimated consequences, and we use estimates of risk to put into perspective the expected detriment associated with these scenarios.

- We calculate the total radiological risk from all significant scenarios using the risk equation prescribed by the AECB, because the main AECB criterion is expressed as a radiological risk limit (AECB 1987a). For most chemically toxic contaminants of interest, data are generally not available to permit calculation of risk. Thus we report estimated concentrations for chemically toxic contaminants and compare these concentrations with regulatory guidelines and other criteria.

- Our analysis is focussed on the estimation of the radiation dose (followed by calculation of radiological risk) to human individuals and not to human populations. This approach follows regulatory requirements established by the AECB, which also specify that the human individuals are members of the "critical group," a hypothetical "group of people that is assumed to be located at a time and place where the risks are likely to be the greatest, irrespective of national boundaries" (AECB 1987a).

- Our estimates of risk use the product of probability and consequence, where probability refers to the probability of a scenario, and consequence refers to a serious health effect caused by exposure to ionizing radiation (CSA 1991, AECB 1987a). In our scenario analysis (Chapter 4), we have identified three types of scenarios that could make a significant contribution to the risk for times up to 10^4 a. All three types of scenarios are analyzed quantitatively for times up to 10^4 a in Chapter 6, to estimate their contributions to the radiological risk.

- Our analysis of the high-probability scenarios uses a probabilistic approach, referred to as systems variability analysis (Dormuth and Quick 1980), which is a method of probabilistic risk (or safety) assessment (ERL 1985, Saltelli 1989, Garrick 1989, Goodwin 1989). Systems variability analysis provides a comprehensive and systematic method for dealing with uncertainties in the estimation of consequences (Sections 2.1 and A.3).

The overall objectives of the postclosure assessment and the specific objectives of its application to the reference disposal system are similar to those of other environmental and safety impact statements. However, it must be noted that the assessment is applied to a hypothetical disposal system and not to a specific project. Thus the results of the study should be appropriately qualified.

There is a second important qualification: this postclosure assessment of the reference disposal system is based on information that would typically derive from an interim study of one potential site during the site evaluation substage but prior to exploratory excavation. Thus the results of the study would contribute to a decision on whether more detailed investigations of the potential site should be performed. Additional postclosure assessments using the more detailed information would contribute to decisions made in subsequent stages.

1.3 SCOPE OF THE POSTCLOSURE ASSESSMENT

1.3.1 Overview of the Concept

The concept for the disposal of Canada's nuclear fuel waste involves deep underground burial in plutonic rock of the Canadian Shield (AECL 1994a). A series of engineered barriers and natural barriers would be used to immobilize and isolate the waste so as to protect human health and the environment.

Figure 1-2 illustrates the main features of the concept. It shows a disposal vault located at depth in a host rock. During operations, a surface facility connects with the vault through a set of access and ventilation shafts. The concept has the following main features:

- the waste would be either used CANDU fuel or solidified highly radioactive reprocessing waste;
- the waste would be sealed in a container designed to last at least 500 a and possibly much longer;
- the containers of waste would be emplaced in rooms in a disposal vault or in boreholes drilled from the rooms;
- the vault would be nominally 500 to 100 m deep;
- the geologic medium would be plutonic rock of the Canadian Shield;
- the waste containers would be separated from the rock by a buffer material;
- each room would be sealed with backfill and other vault sealing materials; and

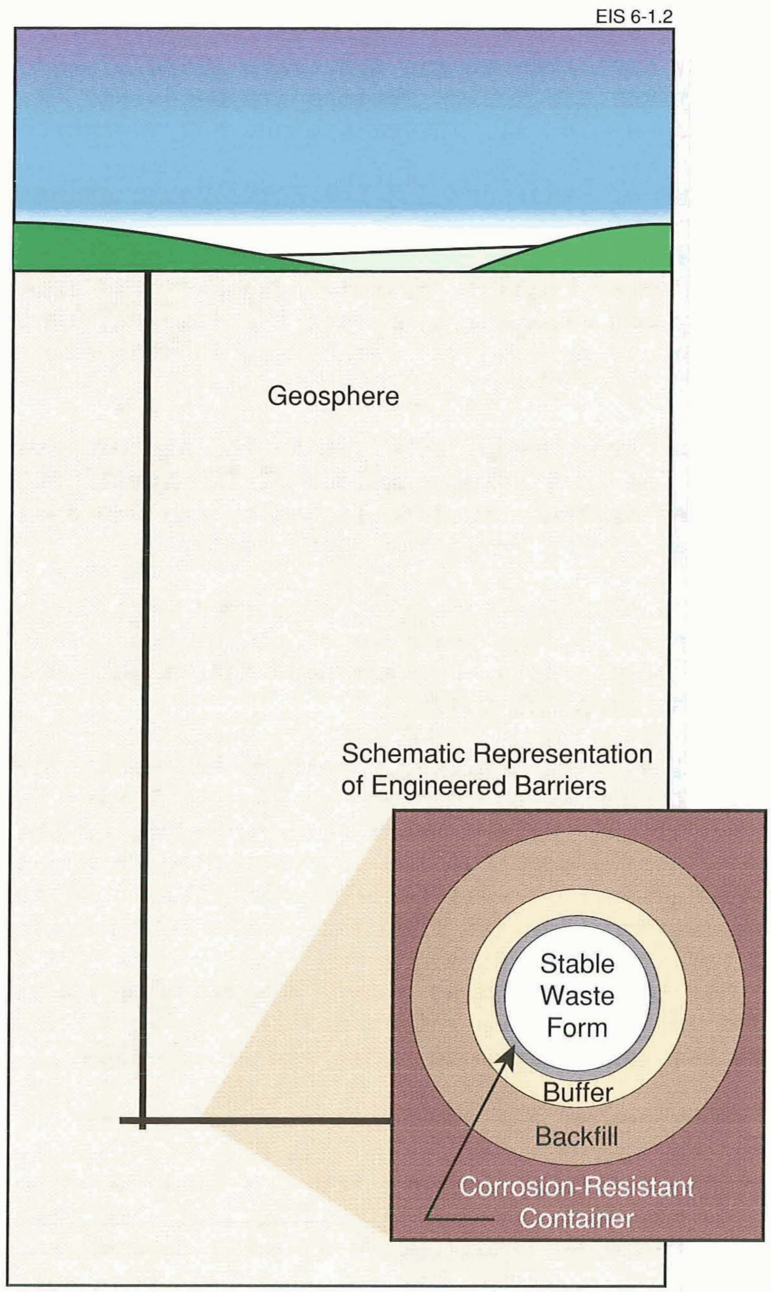

FIGURE 1-2: The Concept for Geological Disposal of Canada's Nuclear Fuel Waste

The concept is based on a system of multiple man-made and natural barriers to isolate the waste from the surface environment. The system should be passively safe for thousands of years.

- all tunnels, shafts, and exploration boreholes would ultimately be sealed such that the system would be passively safe, that is, long-term safety would not depend on institutional controls.

The concept is described in the EIS (AECL 1994a,b) and the engineered barriers alternatives and design options are described in two of the primary references (Johnson et al. 1994a, Simmons and Baumgartner 1994).

1.3.2 Terms of Reference for the Postclosure Assessment

The postclosure assessment is concerned with the potential long-term environmental and safety impacts of this concept. The assessment covers the period that starts from the time when the disposal facility would have been decommissioned and permanently closed and extends thousands of years into the future.

The features of the concept relevant to the postclosure assessment, therefore, concern the long-term behaviour of the waste after the vault rooms would have been filled, the tunnels and shafts would have been sealed, and the surface facilities would have been removed.

The postclosure assessment is also concerned with the entire disposal system. The disposal system consists of the disposal vault and the surrounding geosphere (host rock) and biosphere that might be affected by the presence of the disposal vault.

For the postclosure assessment, we assume that short-duration transients that might follow upon the closure of the vault have ceased and that these transients would not affect the long-term safety of the disposal system. For example, during construction and operation of the disposal vault, some of the surrounding rock will become unsaturated. We assume in the postclosure assessment that the flooding of the vault is complete, so that saturated conditions have been established within the vault and reestablished within the surrounding rock. A discussion of short-term transients is provided in the primary references for the vault model (Johnson et al. 1994b) and the geosphere model (Davison et al. 1994b).

1.3.3 Overview of the Reference Disposal System

The concept describes a disposal facility that could potentially be located somewhere on the Canadian Shield (Figure 1-3). We demonstrate this method for a hypothetical or illustrative disposal system, referred to as the reference disposal system. The reference disposal system generally conforms to the characteristics of the concept, except that specific choices must be made for the various components of the system. For example, the reference disposal system studied in this postclosure assessment comprises a vault, a geosphere and a biosphere, and we have made the following assumptions.

The *reference vault* includes used CANDU fuel bundles, encapsulated in thin-walled titanium containers packed with particulate material for mechanical support, emplaced in boreholes surrounded by a sand-bentonite mixture, in

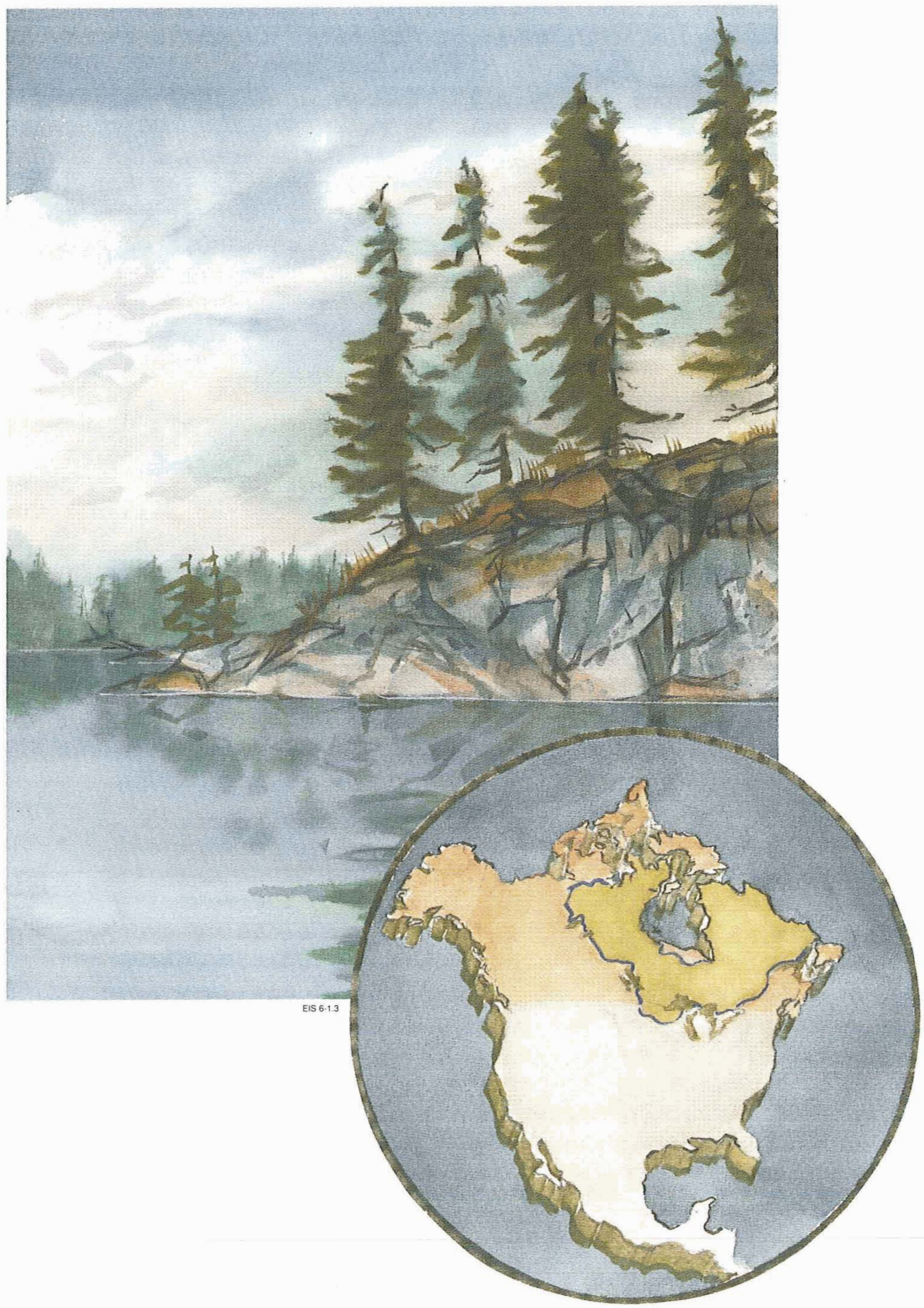

FIGURE 1-3: The Canadian Shield and an Artist's Illustration of a Typical Shield Area

A typical area on the Shield has numerous lakes and rivers with rocky islands and shores. The thin layers of soil host a diversity of plants, such as evergreens and deciduous trees. The Shield is inhabited by people in many widely distributed communities and by a variety of wildlife.

the floor of rooms filled with a backfill of crushed granite and glacial lake clay, and sealed with concrete bulkheads (Johnson et al. 1994b). We assume the vault is located at its minimum nominal depth or 500 m. We also assume the mass of the waste is 162 000 Mg U, although a larger value, 191 000 Mg U, is cited in the primary reference for the conceptual design (Simmons and Baumgartner 1994). The smaller mass used in the reference vault follows from a particular option we chose during the development of derived constraints, described in Section 6.2. We provide more details on the reference vault in the description of its associated model and data (Section 5.2).

The *reference geosphere* consists of the host rock formation, its groundwater flow system, the materials used to seal the shafts and exploration boreholes, and a well used to supply water (Davison et al. 1994b). The geological characteristics of the reference geosphere are derived using data from AECL's studies in the Whiteshell Research Area (WRA), near Lac du Bonnet, Manitoba. This WRA is on the edge of the Canadian Shield and has many features in common with sites elsewhere on the Shield. The WRA includes a large portion of the Lac du Bonnet batholith, a large granitic rock body several kilometres deep with an exposed surface over 60 km long and 20 km across at its widest part. The batholith, the surrounding rocks and the interfaces between them have been the subject of extensive field investigation for more than a decade. A large volume of detailed information about the geology has developed from studies used to locate and construct an Underground Research Laboratory in the WRA. We provide more details on the reference geosphere in the description of its associated model and data (Section 5.4).

The *reference biosphere* consists of the surface and near-surface environment, including the water, soil, air, people and other organisms (Davis et al. 1993). Information from the WRA is used to characterize details such as the location of water bodies and discharge areas of groundwater that might have passed through or near the reference vault. Other, more general information is assumed to be typical of the Canadian Shield, consisting of rocky outcrops; bottom lands with pockets of soil, marshes, bogs and lakes; and uplands with meadows, bush and forests. Changes in climate, surface water flow patterns, soils and vegetation types are expected to be within the range of variation currently observed on the shield and included in the reference biosphere. We provide more details on the reference biosphere in the description of its associated model and data (Section 5.6).

1.3.4 Overview of the Postclosure Assessment Approach

For quantitative estimates of effects, the postclosure assessment makes use of a mathematical simulation approach. Simulations are used to describe the movement of contaminants through the disposal system and to provide estimates of subsequent effects.

The mathematical models and associated data are chosen to represent all features, events and processes that we believe, on the basis of current knowledge and understanding, are important to the postclosure assessment of the reference disposal system. The primary reference for the vault model

(Johnson et al. 1994b) identifies the factors that could affect the long-term performance of the reference vault and justifies of the models and data used to represent important factors. Similarly, the models and data describing the geosphere and biosphere of the reference disposal system are documented in the primary references for the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993).

The models and data used to assess the high-probability scenarios (called the SYVAC scenarios in Chapter 4) are implemented by a computer code known as SYVAC3-CC3. (SYVAC3-CC3 is an acronym for Systems Variability Analysis Code, generation 3, using models for the Canadian Concept, version 3, for the disposal of Canada's nuclear waste; it is described in Section A.3 of Appendix A). This computer code follows an approach known as systems variability analysis and was developed to take into account the uncertainty (including temporal and spatial variability) in the parameters used by the models.

The postclosure assessment provides quantitative estimates of effects for times up to 10^4 a, to meet the regulatory requirements outlined in Section 1.4. Simulations are also carried out for times up to 10^5 a. Results from these extended simulations, along with further analyses based on the geological record and scientific principles, provide qualitative estimates of effects over longer time frames.

Chapter 2 provides more information on the postclosure assessment method; Chapters 3 to 8 describe its application to the reference disposal system.

1.3.5 Application to a Real Disposal Facility

AECL Research has developed a postclosure assessment method and applied it to a study of the reference disposal system. Although this disposal system is hypothetical, it is based on real data and assumptions that are either realistic or conservative.

We believe that this generic method could be used to assess an actual disposal system located at some specific site on the Canadian Shield. The method is relatively flexible. We show, for example, that the collective and individual knowledge of a multidisciplinary group of experts can be successfully integrated into the assessment; that interim postclosure assessments can contribute to the optimization of a disposal design; that major sources of data uncertainty can be taken into account; and that the assessment results can be readily updated to include new research information.

1.4 ENVIRONMENTAL CRITERIA, GUIDELINES AND STANDARDS

One specific objective of the postclosure assessment is to compare estimated environmental impacts with criteria, guidelines and standards set forth by regulatory agencies. This section reviews the criteria, guidelines and standards that would apply to a nuclear fuel waste disposal facility in Canada and indicates where they are used in this report.

Sections 1.4.1 and 1.4.2 examine the protection of human health from radioactive and chemically toxic contaminants that might be released from a disposal vault in the postclosure phase. Section 1.4.3 deals with protection of the environment.

1.4.1 Protection of Human Health from Radioactive Contaminants

In Canada, the AECB is responsible for criteria, guidelines and standards that apply specifically to the operation of nuclear facilities. Three AECB regulatory documents apply to the postclosure assessment, namely R-71 (AECB 1985), R-104 (AECB 1987a) and R-72 (AECB 1987b). Their contents are summarized in Figure 1-4 and in the following text (Appendix C provides more details).

The general requirement in Regulatory Document R-104 (AECB 1987a) is related to radiation dose to individuals in the critical group (this group is defined below). We believe this focus is fitting and note that a similar conclusion has international support:

> Individual dose or risk limits were generally regarded as more appropriate for determination of the long-term acceptability of high-level waste disposal practices than collective dose or risk limits, which should be used mainly as a comparison tool for discussion of vault design alternatives (NEA 1991).

Current Canadian regulatory policy is based on the 1977 recommendations of the International Commission on Radiological Protection (ICRP) (ICRP 1977). In 1990, the ICRP revised its recommendations (ICRP 1991). Section E.2 in Appendix E discusses the implications that the new ICRP recommendations have for the results and conclusions of this postclosure assessment.

Regulatory Document R-71 (AECB 1985)

The AECB Regulatory Document R-71 defines general requirements for a geological disposal system, specific requirements for the concept assessment and its documentation, and specific requirements for the analysis and predictive modelling of the performance of the disposal system. For example, R-71 requires that the postclosure assessment include

- estimates of annual effective dose equivalent, and
- evaluation of the significance of inadvertent human intrusion into the vault.

Chapter 6 describes estimates of annual effective dose equivalent to humans that are attributable to the contaminants placed in the disposal vault. In this report, we use the abbreviation "annual dose" to represent the annual effective dose equivalent, and we report it in units of sieverts per year (Sv/a).

AECB Regulatory Document R-71 defines

- The general requirements for an acceptable disposal facility, for the assessment of the concept and for the analysis and predictive modelling of potential impacts.
- A specific requirement calling for estimates of annual effective dose equivalent and requiring that the probability of doses be "small."

AECB Regulatory Document R-72 describes

- The geological considerations for siting an underground disposal facility for high-level waste.
- Some properties that should be accounted for in the postclosure assessment.

AECB Regulatory Document R-104 presents

- The quantitative criteria for judging the acceptability of a disposal facility and guidelines for preparing the postclosure assessment.
- A specific criterion stating that the radiological risk to the most exposed individuals must be less than 10^{-6} health effects in a year.
- Application guidelines, such as the need to prepare quantitative estimates to 10 000 years following closure, with reasoned arguments for longer times.

FIGURE 1-4: The Atomic Energy Control Board Regulatory Requirements

> Annual dose [to humans] represents the sum, over one year, of the effective dose equivalent resulting from external exposure and the 50-year committed effective dose equivalent from that year's intake of radionuclides (Davis et al. 1993). Thus annual dose determines the estimated biological consequences of internal and external exposures, with corrections accounting for the effectiveness of different types of radiation in causing biological damage and the radiosensitivity of different body organs. In addition, the term "50-year committed" means that internal exposure includes the dose received during the current year plus the dose that would be received over the next 49 years from those radionuclides that may remain in the human body.

Annual dose is calculated for a member of the critical group, a hypothetical group of individuals expected to receive the largest impacts from a disposal system.

Chapter 6 also evaluates the potential impacts associated with inadvertent human intrusion.

<u>Regulatory Document R-72 (AECB 1987b)</u>

The AECB Regulatory Document R-72 is oriented toward considerations for siting a disposal facility. It describes the general characteristics of a disposal facility in terms of fundamental objectives and requirements, including the use of engineered and natural barriers to

- isolate and retain radioactive contaminants,
- restrict their movement from the disposal vault, and
- restrict human access to the waste.

The AECB Regulatory Document R-72 notes that the system must be "capable of accommodating disturbances due to natural phenomena likely to occur in the vicinity of the vault" and that the "disposal should be passive; that is, it should be designed to minimize the obligation imposed on future generations to oversee the continued safe isolation of the waste." (AECB 1987b).

We deal with these issues as follows.

- Section 6.4 (and elsewhere in Chapter 6) provides a quantitative description of the effectiveness of engineered and natural barriers in isolating and retaining contaminants and in restricting the movement of contaminants that may escape from the disposal vault.
- Chapter 8 presents an overall summary of the effectiveness of the disposal system in restricting human access to the waste, based on the detailed evaluations in Chapters 6 and 7.

- Chapters 4, 6 and 7 discuss the ability of the disposal system to accommodate disturbances and to operate in a passive mode. More details are provided in the EIS (AECL 1994a) and in the primary references for the geosphere model (Davison et al. 1994b), site screening (Davison et al. 1994a), the vault model (Johnson et al. 1994b), the biosphere model (Davis et al. 1993), the engineered barriers (Johnson et al. 1994a) and the conceptual design (Simmons and Baumgartner 1994)).

Regulatory Document R-104 (AECB 1987a)

The AECB Regulatory Document R-104 presents three basic requirements: minimize the burden on future generations, implement a disposal option "in a manner such that there are no predicted future impacts on the environment that would not be currently accepted and such that the future use of natural resources is not prevented," and protect human health (AECB 1987a). This third requirement contains a quantitative criterion for the post-closure phase:

> The predicted radiological risk to individuals from a waste disposal facility shall not exceed 10^{-6} fatal cancers and serious genetic effects in a year, calculated without taking advantage of long-term institutional controls as a safety feature.
>
> . . . risk is defined as the probability that a fatal cancer or serious genetic effect will occur to an individual or his or her descendants. Risk, when defined in this way, is the sum over all significant scenarios of the products of the probability of the scenario, the magnitude of the resultant dose and the probability of the health effect per unit dose.
>
> . . . a risk of 10^{-6} in a year is the risk associated with a dose of 0.05 mSv in a year (AECB 1987a).

This associated annual dose (0.05 mSv/a) also corresponds to the de minimus dose of radiation to individuals (AECB 1989).

The AECB Regulatory Document R-104 additionally provides four guidelines that pertain to the postclosure assessment.

Guideline 1 - Identifying the Individual of Concern

> The individual risk requirements in the long term should be applied to a group of people that is assumed to be located at a time and place where the risks are likely to be the greatest, irrespective of national boundaries [Guideline 5.1 (AECB 1987a)].

Guideline 2 - Probabilities of Exposure Scenarios

> The probabilities of exposure scenarios should be assigned numerical values either on the basis of relative frequency of occurrence or through best estimates and engineering judgments [Guideline 5.2 (AECB 1987a)].

Guideline 3 - Timescale of Concern

> The period for demonstrating compliance with the individual risk requirements using predictive mathematical models need not exceed 10,000 years. Where predicted risks do not peak before 10,000 years, there must be reasoned arguments leading to the conclusion that beyond 10,000 years the rate of radionuclide release to the environment will not suddenly and dramatically increase, . . . acute radiological risks will not be encountered by individuals . . . and major impacts will not be imposed on the biosphere [Guideline 5.3 (AECB 1987a)].

Guideline 4 - Output from Predictive Modelling

> Calculations of individual risks should be made by using the risk conversion factor of 2×10^{-2} per sievert and the probability of the exposure scenario with either:
>
> (a) the annual individual dose calculated as the output from deterministic pathways analysis; or
>
> (b) the arithmetic mean value of annual individual dose from the distribution of individual doses in a year calculated as the output from probabilistic analysis [Guideline 5.4 (AECB 1987a)].

The postclosure assessment of the reference disposal system includes an estimate of the radiological risk that complies with these four guidelines.

Much of our analysis is focussed on estimates of a variable that is measurable: annual dose to members of the critical group. We then use these estimates to calculate the radiological risk, using the prescribed equation:

$$\text{Risk} = \sum_i p_i \, d_i \, k \qquad (1.1)$$

where the summation extends over all significant scenarios and where

p_i is the probability of occurrence of scenario i (Guideline 2);

d_i is the annual dose (annual effective dose equivalent in Sv/a), as specified in R-71, to an individual in the critical group (Guideline 1) and is the estimate for scenario i; and k is the risk conversion factor, a constant whose numerical value is 2×10^{-2} serious health effects per sievert (Guideline 4).

The unit of risk is probability of serious health effects in a lifetime per year of exposure.

In considering the requirements of R-104, we note the following points.

- Guideline 4 allows that calculations of risk can be made using a single estimate of annual dose, following deterministic pathways analysis or using many estimates of annual dose, following probabilistic pathways analysis. If a probabilistic analysis is followed, d_i in Equation 1.1 should be the arithmetic average of the estimated annual dose.

  Although our analysis provides both a single estimate and an arithmetic average (from many estimates) of annual dose, we consider the latter to be more informative for the decision-making process. Probabilistic analysis includes the effects of parameter uncertainty and variability, and we show in Section 6.5.1 that uncertainty has significant effects on the results of the postclosure assessment of the reference disposal system.

- Guideline 1 describes the general characteristics of the individuals of concern who make up the critical group. We have defined the behaviour of these individuals such that they would be exposed to the greatest risk. For example, we assume that the individuals spend their entire lives in an area where they would be exposed to the groundwater potentially contaminated by the disposal vault and that they obtain all their food, water, fuel and building materials from this area. Section 5.6 and the primary reference for the biosphere model (Davis et al. 1993) provide more details on the characteristics of the critical group.

- From our analysis of exposure scenarios (Guideline 2), we identify three types of scenarios that require quantitative evaluation for the postclosure assessment of the reference disposal system. Our analysis, discussed in Chapters 4 and 6, includes consideration of their probabilities of occurrence and their potential impacts.

- Finally we address Guideline 3 by providing quantitative estimates of annual dose and radiological risk to 10^4 a following closure; our results are documented in Sections 6.5, 6.7 and 6.8. Because annual dose (and risk) does not peak in this time frame, we provide in Chapter 7 reasoned arguments describing critical aspects of the expected performance of the disposal system for times far beyond 10^4 a. (More general arguments are presented in the EIS (AECL 1994a).) These results are also summarized in Section 8.2.

1.4.2 Protection of Human Health from Chemically Toxic Contaminants

The AECB Regulatory Documents R-71 and R-104 (AECB 1985, 1987a) specify that environmental impacts must be assessed for both radioactive and non-radioactive contaminants released from the disposal facility. These documents supply a risk criterion for radioactive contaminants but no equivalent criteria for nonradioactive contaminants.

For the postclosure assessment of the reference disposal system, we have taken into consideration Canadian regulations and guidelines currently available for contaminants in soil, water and air. Where no regulations and guidelines are available, we have developed guidelines that would ensure that impacts would not be overlooked.

For example, for contaminant concentrations in water, we use the most stringent of the regulations and guidelines from these sources: *Guidelines for Canadian Drinking Water Quality* (Health and Welfare Canada 1989), *Water Quality Sourcebook* (McNeely et al. 1979), and *Metal Mining Liquid Effluents Regulations* (Government of Canada 1978); we also examined regulations in the *Ontario Water Resources Act* (Government of Ontario 1978) and in the *Environmental Protection Act of Ontario* (Government of Ontario 1980). These sources were used to determine the most restrictive guideline for each chemical element of concern.

Where an element is not covered by a regulation or guideline, we assume a concentration guideline that is expected to have a large margin of safety. The assumed limit is based on information such as concentrations found in nominally uncontaminated groundwaters of the Canadian Shield, toxicity data for ingestion, and arguments based on chemical analogy (Goodwin and Mehta 1994).

The postclosure assessment of the reference disposal system provides estimated concentrations of contaminants in air, water and soil in the local habitat of the critical group for comparison with regulations and guidelines. We calculate and report (in Section 6.5.3) the arithmetic averages of these concentrations, using results from the probabilistic pathways analysis. As in the case for the average annual dose, we consider the probabilistic pathways analysis to be more valuable for decision making because it includes the effects of parameter uncertainty.

1.4.3 Protection of the Environment

The regulations described in Sections 1.4.1 and 1.4.2 are mostly oriented toward protecting human health. However, R-104 (AECB 1987a) states that "there is also a need to provide adequate protection for the general environment from the impacts that might arise from either radioactive or non-radioactive contaminants" (AECB 1987a). The Environmental Review Panel has also highlighted a requirement for protection of the environment in its guidelines (EARP 1992).

We have not identified any well-recognized criteria, standards or guidelines that could be used to compare with our estimates of impact on the environment. Therefore, we have followed the methodology discussed by

Amiro (1992a, 1993) and Davis et al. (1993), which conforms with similar studies on protection of the environment. We compare estimated concentrations of radioactive and nonradioactive contaminants with baseline concentrations of the same contaminants that currently exist on the Canadian Shield. We assume that a contaminant from the disposal facility is environmentally acceptable if its estimated concentration falls within the *variability* of its background concentration in the natural environment.

We use this test to identify contaminants that are of potential concern for protection of the environment. We then evaluate the potential effects of these contaminants. Section 6.5.4 documents these results.

Potential effects include estimates of dose to members of the critical group and to other organisms. In the postclosure assessment, we assume that the critical group inhabits the most contaminated parts of the environment. If the estimated annual dose to the critical group is small, then the annual doses to other species are also likely to be small. However, nonhuman organisms could be exposed to larger doses because of ecological differences and, for this reason, we also estimate radiation dose to representative nonhuman biota. Comparisons are made with available environmental baseline data from the Canadian Shield to evaluate the expected severity of the impacts to nonhuman biota.

2. THE POSTCLOSURE ASSESSMENT APPROACH

2.1 CONTENTS OF THIS CHAPTER

In this chapter, we describe the postclosure assessment method developed to conform with the objectives, scope and regulatory requirements described in Chapter 1.

Sections 2.2 to 2.5 describe the method used for the quantitative analysis. This method is then applied to an illustrative disposal system that we refer to as the reference disposal system. Results of the application, documented in Chapters 3 to 6, are focussed on the first 10^4 a following closure of the reference disposal facility.

Section 2.6 outlines the method used to analyze the system over longer time frames. The corresponding results for the reference disposal system are documented in Chapter 7.

2.2 IMPORTANT REQUIREMENTS FOR THE ASSESSMENT APPROACH

The following considerations have had a strong influence on the development of a quantitative method for the postclosure assessment:

1. *The postclosure assessment must provide quantitative estimates of effects over long time frames.* The AECB requires quantitative estimates of impacts for 10^4 a following closure of the disposal system and reasoned arguments covering the performance of the disposal system for times beyond 10^4 a (AECB 1987a).

2. *An acceptable disposal system must meet the AECB regulatory criterion of a small radiological risk to human health.* The AECB has set a general requirement on radiological risk to an individual of 10^{-6} fatal cancers and serious genetic effects per year for times up to 10^4 a (AECB 1987a). This risk is associated with an annual dose of 5×10^{-5} Sv/a (AECB 1987a). For comparison, radiation in the natural environment is typically about 3×10^{-3} Sv/a (Neil 1988), or about 50 times greater. Thus our quantitative analysis must be capable of estimating radiation doses that are much smaller than those that now exist from naturally occurring sources in the environment.

3. *The CNFWMP is in the concept assessment stage, but we endeavour to use models and data that are as realistic as possible for the quantitative assessment.* The assessment at this stage must deal with a concept, not an actual disposal facility at a particular site (AECL 1994a). Therefore, we must satisfy the requirement to prepare quantitative estimates of effects despite the necessity of basing the assessment on a disposal system that is still in the conceptual stage. Because an actual site and facility do not exist, we must make some assumptions for information not yet available and for options not yet chosen. There is an implied constraint in these assumptions: the performance of the disposal system is strongly dependent on its characteristics, and these characteristics should not be arbitrarily generated. Rather, the models and data must be internally consistent and based, to the extent possible, on real information from actual observations.

4. *Where it is not possible to be realistic, we make simplifying assumptions that lead to an overestimate of impacts.* The use of conservative models and data is appropriate because our primary goal is to show the disposal system meets established safety criteria, rather than to predict future behaviour.

2.3 QUANTITATIVE ESTIMATES OF IMPACTS

Because the disposal system is designed to protect humans and the environment for tens of thousands of years, we cannot base the quantitative assessment on actual observations of its long-term performance. Thus we use scientific arguments and simulations with mathematical models to infer the long-term behaviour of the disposal system and to estimate its potential effects. These effects are discussed in Chapter 6, where we describe an application of the method to an assessment of the reference disposal system.

Some features of this system are specified in detail; others must remain general. For example, we use a specific design and location for the hypothetical vault because our research indicates that a generic design and location would not provide useful and realistic results (Davison et al. 1994b). On the other hand, we can assume a more general surface environment and a range of characteristics of the affected human population (Davis et al. 1993, Zach and Sheppard 1992, Bird et al. 1992, Sheppard 1992).

The postclosure assessment method is based on the six steps shown in Figure 2-1. An important element of the method, not explicitly shown in the figure, is the extensive feedback between all steps. That is, it may be necessary to modify the work carried out in an earlier step as a consequence of preliminary studies of a following step. We emphasize this point with an example. In the scenario analysis (step 2), we identified gases, such as hydrogen, as possible agents that could enhance contaminant transport in the vault and geosphere. Subsequent consideration of available models and data (step 3) showed that there is little detailed information available on gas-induced transport. We addressed this issue by modifying the specifications of the reference disposal system (step 1) as follows:

- Most of the hydrogen gas would be generated from corrosion of iron or steel separators included in the original container design. We subsequently assumed that the container design for the reference disposal system precluded the use of iron or steel. With this modification, Johnson et al. (1994b) show that a gas phase could not occur for at least 2 x 10^4 a. Thus there is no need to include any transport-induced effects caused by hydrogen gas in the quantitative modelling to 10^4 a for the containers in the reference disposal system. (However, there is a need to consider possible effects for times beyond 10^4 a.)

Section 6.2 describes another important example of feedback: a preliminary study (from steps 4 and 5) points to a modification of the layout of the vault (step 1) that greatly improves the margin of safety of the reference disposal system.

In the remainder of this section, we outline each of the six steps of the assessment method (Figure 2-1) and note where further details may be found.

2.3.1 Specify System Features

In the first step of the study, we describe the reference disposal system to provide the basis for this postclosure assessment.

The concept for disposal of Canada's nuclear fuel waste involves isolation of the waste in plutonic rock of the Canadian Shield. A complete description of the concept, given in the EIS (AECL 1994a), allows many possible options and alternatives. However, the postclosure assessment of the reference disposal system is focussed on a specific design and a specific site.

Chapter 3 summarizes the characteristics of the reference disposal system assessed in this report. Additional details are described elsewhere; for example, Section 5.4 describes the assumed hydrogeology and Section 6.2 documents a preliminary analysis that affects the engineering design and layout of the reference disposal vault.

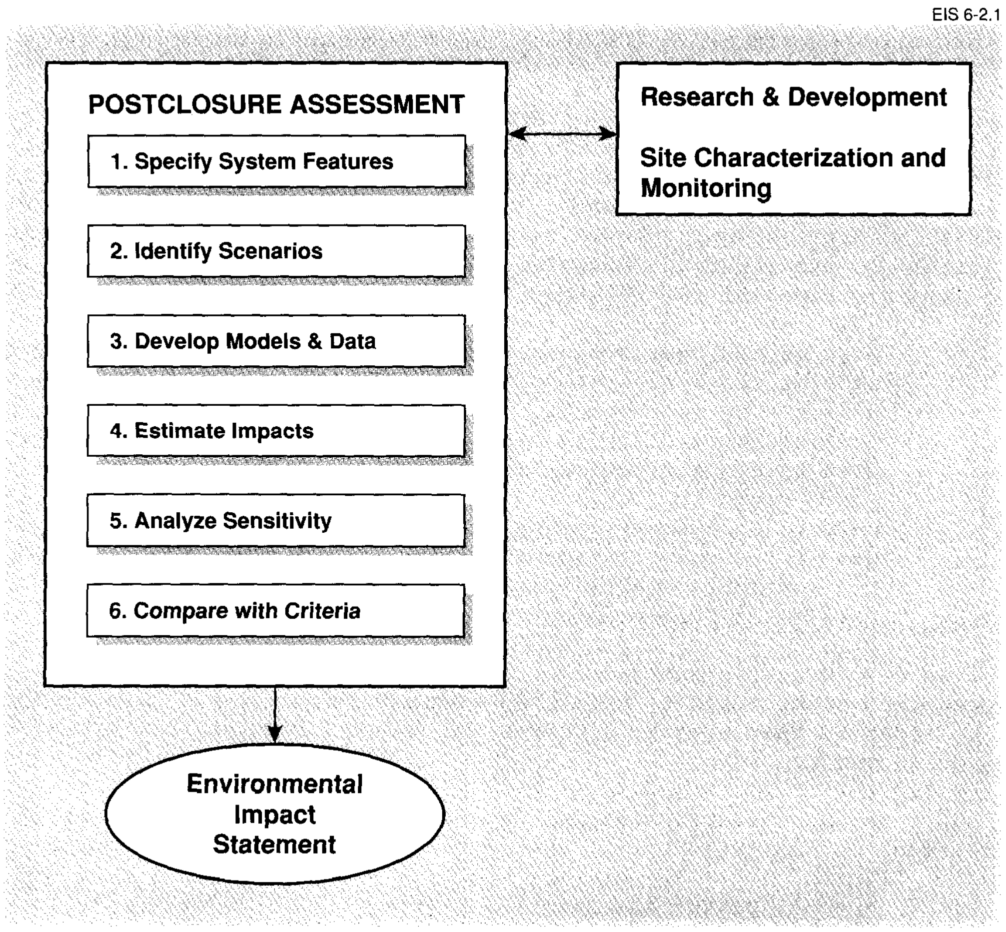

FIGURE 2-1: The Steps in the Simulation Approach for the Postclosure Assessment

In the first step, we specify the features of the system or case study to be evaluated in the postclosure assessment; for example, we stipulate the particular vault design and container material to be assessed from among the possible options. We then identify all scenarios warranting quantitative evaluation. In steps 3 and 4, we develop the models and data required to simulate the long-term behaviour of the disposal system and to estimate potential impacts. We apply sensitivity analysis in step 5 to identify important elements that could affect safety and performance. In the last step, estimated impacts are compared with regulatory criteria, standards and guidelines. The results are then documented in the environmental impact statement.

In applying this approach, there may be considerable feedback between steps. That is, the results and conclusions from one step may bring about some changes and decisions that require repetition of another.

This figure also indicates that there is a strong interplay between the postclosure assessment and the supporting program for research and development, site characterization and monitoring. This interplay enters into all steps of the assessment approach.

2.3.2 Identify Scenarios

In step 2, we systematically identify all factors that could significantly affect the future performance of the disposal system.

Factors may be classified as features, events and processes; examples include features such as the presence of fracture zones in the rock surrounding the disposal vault, events such as glaciation and earthquakes, and processes such as container corrosion mechanisms and the diffusion of contaminants in groundwater.

We then decide how these factors should be taken into account in the postclosue assessment. Two time frames are considered, in keeping with the requirements of the AECB (1987a).

- Many factors require quantitative evaluation because they could affect estimates of impacts for times up to 10^4 a following closure of the disposal system.

- Some additional factors require evaluation using reasoned arguments because they may have significant effects for times beyond 10^4 a.

Some factors would not have significant effects on either time-scale. One example is the possible assembly of a critical mass of fissile material in the disposal vault, leading to a self-sustaining fission reaction. McCamis (1992) concludes that the occurrence of this process is not credible, and thus it does not require further consideration in the postclosure assessment. We document why all such factors are not considered further.

Factors that require quantitative evaluation are assembled into scenarios that describe possible future states and behaviour of the disposal system. We then evaluate these scenarios and estimate their impacts. For the reference disposal system, we conclude that quantitative evaluation is required for three types of scenarios for times up to 10^4 a.

- The first type of scenarios involves groundwater-mediated processes that are expected to occur: corrosion of the containers, release of contaminants from the nuclear fuel waste, movement of contaminants through the vault seals and surrounding rock by diffusion and by transport in slowly moving groundwater, and eventual discharge of contaminants at the surface where they may result in environmental impacts. We refer to these scenarios as the SYVAC scenarios because their potential impacts are evaluated using simulations with the mathematical models contained within the computer code SYVAC3-CC3 (see Section A.3 of Appendix A).

- The second type of scenarios requiring evaluation is called the open-borehole scenarios. These scenarios describe a situation for the reference disposal system in which one or more open boreholes pass close to a vault room containing nuclear waste. Although this situation is expected to be unlikely, it could provide an important alternate pathway for the movement of contaminants from the reference disposal vault to the biosphere.

- The third type of scenarios is referred to as the inadvertent human intrusion scenarios. These scenarios describe a situation in which there is a major disruption of the integrity of the reference disposal system. We assume in our studies that these scenarios are initiated by an activity such as a drilling operation which leads to the direct removal of nuclear waste from the reference disposal vault and dispersion of this waste in the biosphere.

Most of the factors in these scenarios also require evaluation for times beyond 10^4 a, together with some additional factors that could be significant over very long time-scales.

The results of scenario analysis for the reference disposal system are described further in Chapter 4. (Details of the methodology for scenario analysis are given by Goodwin et al. (1994) and are summarized in Section A.2 of Appendix A.) It should be noted that the scenario analysis described in this document applies only to the reference disposal system. Similar analyses would be required for different designs and geological settings.

2.3.3 Develop Models and Data for Simulating the System

In step 3, we assimilate all relevant information and data that would apply to the long-term safety of the reference disposal system, and then construct mathematical descriptions (models) for use in preparing conservative estimates of impact.

We relate observations to underlying knowledge and understanding, and then we represent this understanding using mathematical models. These models represent the factors identified as important for each of the scenarios requiring quantitative evaluation and provide the basis to evaluate future behaviour.

Although the reference disposal system is hypothetical, its performance is highly sensitive to the site and design characteristics. We have, therefore, based our models on real observations and data whenever possible. In developing the models and data for the SYVAC scenarios, we have assumed that many characteristics of the reference disposal system conform with observations and information from the WRA. In particular, the model describing the geosphere includes the consistent set of information and data that were available in 1985 on geological and hydrological features of the WRA. The hypothetical reference disposal system also includes a number of other assumptions, such as the depth and dimensions of the disposal vault, the properties of the metallic containers enclosing the waste, and the characteristics of the human population expected to be most at risk.

The models contain parameters that characterize the important features of the reference disposal system. The values selected for the parameters are a reflection of the scientific literature and our observations and measurements from field and laboratory studies. Figure 2-2 illustrates some of

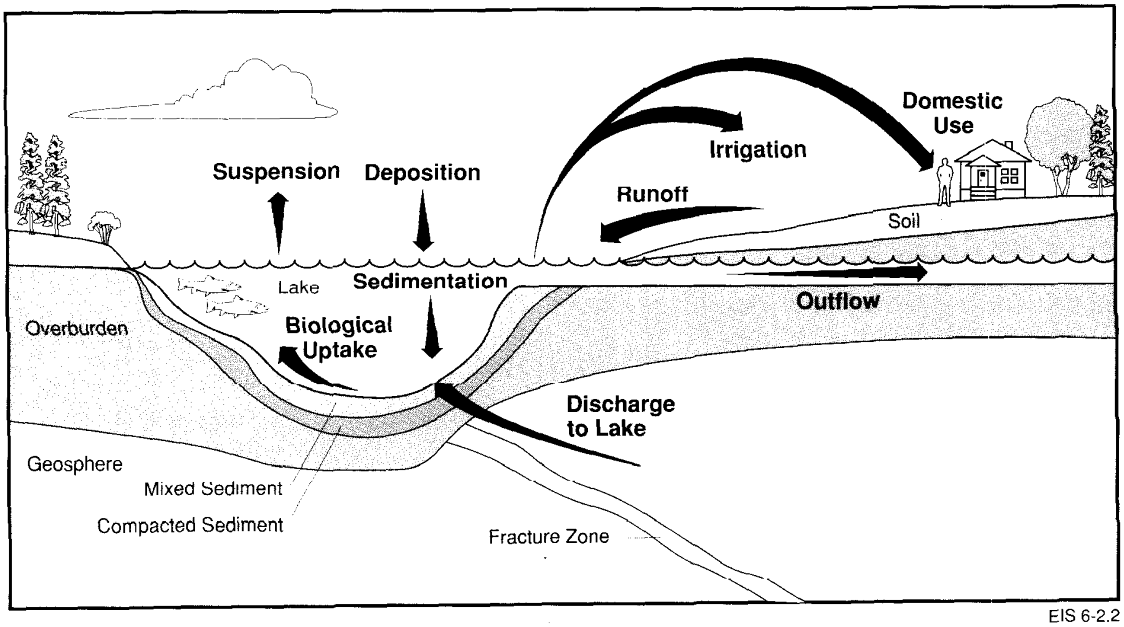

FIGURE 2-2: Features and Processes Used in the Development of a Model

This diagram illustrates features and processes relating to the transport of contaminants into and within a lake. The arrows show mechanisms that may affect the movement of contaminants into or out of the body of water; these mechanisms are described using mathematical equations and several related parameters. For example, "discharge to lake" describes the flow of contaminants into the surface water body from contaminated groundwater. This discharge is modelled using a mass balance equation and parameters that give the rate at which groundwater enters the lake, concentrations of contaminants in that groundwater, and characteristics of the lake sediment layers affecting contaminant retention.

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the features and processes in the system that are represented by the parameters in the biosphere model for the SYVAC scenarios. In many cases, it is not possible to provide precise values for a parameter; consequently, we allow for ranges of possible parameter values that can be used by the models.

In constructing these models (and specifying associated data), our goal has been to provide a realistic and quantitative description of the expected behaviour of all parts of the disposal system. This has not always been practical or feasible: in some instances there may be insufficient information, and in other instances it may be desirable to condense detailed research models and data. In these cases, we have introduced conservative assumptions whose overall effect is to overestimate impacts. That is, the models and data, and the associated set of conservative assumptions, are designed to simulate the movement of contaminants in the reference disposal system in such a way that the study would not underestimate the expected impacts.

We outline in Chapter 5 the models and data used to simulate the reference disposal system for the SYVAC scenarios. More details are provided in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993). Sections 6.7 and 6.8 summarize the models used with the open-borehole and inadvertent human intrusion scenarios.

2.3.4 Estimate Impacts Using Mathematical Simulations

In step 4, we use the models and data to simulate the expected long-term behaviour of contaminants and to estimate the effects of the reference disposal system.

Our analyses of the reference disposal system correspond to a risk analysis, as defined and discussed in Section 1.2:

> Risk analysis is a structured process that attempts to identify both the extent and likelihood of consequences associated with [technological] hazards (CSA 1991).

Chapter 6 documents results for the analysis of the reference disposal system for the scenarios requiring evaluation. For the most part, our analyses are focussed on estimates of radiation dose and concentrations of contaminants in the environment. We then use these more fundamental and measurable quantities to calculate risk using the radiological risk equation (AECB 1987a).

In our analyses of the SYVAC scenarios, we examine both a single simulation and many thousands of randomly sampled simulations. We use the term "deterministic analysis" to refer to the study of a single simulation and "probabilistic analysis" to describe the study of the randomly sampled simulations.

In the deterministic analysis, we focus on a single simulation in which each parameter in the system model is given its median value. The median value is a central value for a parameter that has a distribution of possible values. More precisely, the median is the 50^{th} percentile or 0.5 quantile: if a parameter were randomly sampled 1000 times, about 500 values would be larger and about 500 would be smaller than its median value. Because it is focussed on just one particular simulation, we put little emphasis on estimates of impacts from the deterministic analysis. Instead, we use the deterministic analysis primarily to gain insight into the operation and interactions of the system model.

Probabilistic analysis provides a comprehensive and systematic method for dealing with parameter uncertainties (including spatial and temporal variabilities) in the estimation of impacts (Dormuth and Quick 1980, ERL 1985, Saltelli 1989, Garrick 1989, Goodwin 1989). We follow an approach known as systems variability analysis (Dormuth and Quick 1980), incorporated within the computer code SYVAC3-CC3. In this analysis, we perform thousands of simulations, each having a different set of values for the parameters. Each parameter value is randomly sampled from its allowed distribution of possible values, where the possible values are described using a probability density function (PDF).

For example, in the postclosure assessment of the reference disposal system, the parameter named PRECIP represents the annual precipitation at the reference disposal site; it is described using a normal (or Gaussian) PDF whose mean value is 0.78 m/a and whose standard deviation is 0.11 m/a (Davis et al. 1993). In each of these simulations, a different value of PRECIP is selected at random from its PDF. When thousands of randomly sampled simulations are performed, the values selected for PRECIP would encompass virtually its full range of feasible values, and the corresponding estimated effects would then encompass the full range of possible effects.

The assignment of a PDF for each parameter is made by qualified experts and takes into account the uncertainties in values resulting from the long time-scale of the assessment and the lack of precise and complete data (Stephens et al. 1989, 1993). The primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993) describe the choice of PDF made for each parameter and provide justification for that choice.

The value of a parameter may also be uncertain because of spatial and temporal variability, and its PDF may also include this source of uncertainty. For example, there may be considerable differences in permeability at different locations in a typical granite pluton. That is, the pluton exhibits spatial variability in its permeability. In evaluating the movement of water and contaminants in this rock, it may be necessary to define an "effective" permeability parameter whose possible values are represented by a suitable PDF. This effective parameter actually represents a lumped or averaged quantity that takes into account spatial variability. Its PDF does not directly represent the spatial variability in permeability but, rather, it represents our uncertainty (or lack of knowledge) about the effective values that would account for this variability and other sources of uncertainty.

There may be enough information available to resolve some of the spatial (or temporal) variability. In the case of permeability, information may be available that indicates it takes on small values in one region of the pluton and larger values elsewhere. If the data were sufficient, it may be appropriate to define several smaller volumes of rock, each of which would be characterized by an effective permeability with a unique PDF. These PDFs would incorporate the residual spatial variability of the smaller volumes of rock.

When a site is first studied, it may be described on a relatively coarse scale, with a large amount of spatial variability included in the PDFs of the model parameters. As more details of the site become available, the models and data would be refined and some of the spatial variability would be resolved. The way in which a model is defined and the number of parameters it uses clearly depend on the amount of information that is available. The use of PDFs to represent spatial (and temporal) variability requires the judgment of qualified experts.

At this point, no distinction is made between uncertainty caused by spatial and temporal variability and uncertainty caused by lack of knowledge. From the point of view of the decision maker, both contribute to uncertainty about environmental effects and, therefore, both should be included in the assessment. The distinction would arise when we attempt to reduce the uncertainty in a parameter's values. By way of example, sensitivity analysis may identify a parameter whose uncertain values have a strong influence on the estimates of radiation doses, and it may be possible to reduce the degree of uncertainty that comes from lack of knowledge by conducting further research. However, it may not always be possible to reduce the degree of uncertainty resulting from spatial or temporal variability. (In Section E.7 in Appendix A, we examine how reducing the degree of uncertainty of a parameter can affect estimated impacts.)

The deterministic and probabilistic analyses provide complementary information on the behaviour of the system, and both help to assess the potential effects of the disposal system. Deterministic analysis provides insight into how and where contaminants move within the system, whereas probabilistic analysis provides a powerful technique to include the effects of parameter uncertainties. Chapter 6 summarizes the results of our deterministic and probabilistic analyses for the SYVAC scenarios, with additional details provided in Appendices D and E.

2.3.5 Analyze the Sensitivity of System Performance

In step 5 of Figure 2-1, we perform sensitivity analyses in which parameter values are systematically varied and the models altered, followed by observation and evaluation of changes in the estimated impacts.

Sensitivity analysis is particularly helpful in improving our understanding of the performance of the disposal system. We are also interested in identifying those parameters that have the most effect on potential impacts as their values change from one simulation to another.

One important use of the resulting information is to identify potential derived constraints on the disposal system being studied. A derived constraint is a feasible siting or engineering restriction that could be imposed so that a disposal system would better comply with regulatory criteria and guidelines and provide a greater margin of safety. Section 6.2 describes derived constraints pertaining to the reference disposal system. Section 6.6 documents an extension of this analysis.

The techniques of sensitivity analysis would also be applicable to further studies aimed at improving and optimizing the overall performance of an actual disposal system.

We have developed and applied a sensitivity-analysis technique that can deal with the complex models used to represent the reference disposal system. The technique, called iterated fractional factorial design, is described in Section A.4 in Appendix A. The results of its application are summarized in Chapter 6 with more details in Appendices D and E.

2.3.6 Compare Estimated Impacts with Regulatory Requirements

In this last step, we compare estimated impacts with regulatory criteria, standards and guidelines.

One of the impacts of concern is the annual radiation dose to members of the critical group. The corresponding criterion is expressed as a radiological risk limit, which is associated with an annual dose of 5×10^{-5} Sv/a (AECB 1987a).

We also consider chemically toxic contaminants associated with the nuclear fuel waste and compare their estimated impacts with criteria and guidelines for soil and water used by the critical group. Finally, we examine a broader issue: protection of the environment, including potential radiation doses to nonhuman biota.

In comparing estimated impacts with regulatory criteria, standards and guidelines, we use results from the probabilistic analysis (for the SYVAC scenarios). Our studies show that parameter uncertainty has a strong influence on estimates of impacts for the reference disposal system, and the probabilistic analysis takes into account the effects of these uncertainties.

2.4 REFINING THE MODELS, DATA AND ASSESSMENT APPROACH

The postclosure assessment approach described in Section 2.3 is the product of continuous development and refinement occurring over more than a decade. A preliminary assessment study, completed in 1981 (Wuschke et al. 1981), concentrated on developing models and data for estimating impacts using a simpler representation of the disposal system. This led to enhancements to the method of probabilistic analysis. Subsequent studies (Wuschke et al. 1985, Goodwin et al. 1987b) led to further advances: notably, improvements in the models describing the disposal system (Johnson et al. 1994b, Davison et al. 1994b, Davis et al. 1993) and development of approaches for sensitivity analysis (Walker 1986, Frech and Andres 1987, Andres and Hajas 1993).

The assessment study described herein is the third such study in which the reference disposal system, its representation in the system model and data, and the assessment approach have all been refined as a result of ongoing research and a better understanding of system performance factors. Although we anticipate that further refinements will occur, the assessment results described in this report are based on one particular design of a disposal system and on up-to-date research results and assessment methods. (Section 8.2.6 examines the effects of research information that became available after the quantitative analysis for this assessment was completed.)

In an actual implementation of a waste disposal facility, the observational approach will be used as the project proceeds through the stages of site characterization, construction and operation. As new information, knowledge and understanding are generated, the safety analyses—and the hypothesis, models and data on which they are based—will become increasingly robust. Thus the final assessment would draw from the understanding and data acquired through many decades of studies. The final assessment would also be supported and guided by the results of all earlier assessment studies.

There are several reasons for introducing refinements to the models and data. One is to ensure that the models and data reflect accurately the latest knowledge from the research and site evaluation and monitoring programs. Three other reasons are associated with the information generated by the assessment itself. This information can

- *Test the models and data.* Test results are examined in detail and lead to refinements, corrections and improvements.

- *Point to issues that require further study.* Sensitivity analysis can identify components of a model and its data that have a significant influence on estimated impacts. This information can help guide further investigations, and lead to more reliable and more credible safety analyses.

- *Improve the system performance.* If an estimated impact would not meet a criterion or did not allow a sufficient margin of safety, we would use information from the sensitivity analysis to develop derived constraints on the reference disposal system. Section 6.2 describes analyses that identify potential derived constraints that would increase the margin of safety of the reference disposal system. We have selected a derived constraint related to the vault design, with feedback that necessitated modifications to some design details and their representation in the models and data. For an actual disposal facility, similar studies would contribute to optimizing its performance and cost effectiveness.

2.5 DEALING WITH UNCERTAINTY

In estimating the effects of the disposal system, it is necessary to deal with uncertainty in our understanding of the system's behaviour. Three strategies can be distinguished:

- The best strategy would be to eliminate uncertainty, but this is not feasible, even in principle, for the assessment of the reference disposal system. Nevertheless, some features of the system are so well understood and quantified that we can assume a negligible degree of uncertainty in representing them. An example of such a feature is radioactive decay.

- In the best practical strategy, the effects of uncertainty would be quantified and related to the performance of the disposal system. Many features of the reference disposal system fall into this category; for example, the actual chemical conditions around each container cannot be known precisely, but the effects of their uncertainty can be estimated (Johnson et al. 1994b).

- Finally, if the effects of uncertainty cannot be quantified, then we ensure that the estimates are conservative; that is, that the impacts are overestimated. Several features of the reference disposal system have an uncertainty whose effects cannot be readily quantified, and a conservative assumption is made instead. One example is the critical group's assumed diet that would likely include food produced at some location not affected by the disposal system. Because it would be difficult to quantify and justify this possibility, we make the conservative assumption that the critical group obtains all of its food and water from local sources and that these local sources are within the projected discharge zones of the reference disposal system (Davis et al. 1993).

In the discussion that follows, we explore in more detail the effects of uncertainty and note how they are dealt with in the assessment approach (see also Davis et al. 1990).

2.5.1 Scenarios

One potential uncertainty in defining the reference disposal system is the omission of some unrecognized factors that could have important effects. To minimize this possibility, we have applied a systematic procedure called scenario analysis (Chapter 4 and Section A.2 in Appendix A). The procedure includes continuing surveys of scenario analyses performed for related projects in other countries, scrutiny of issues arising from all elements of the research program and from interactions with the public, and frequent reviews by appropriate technical experts from a wide range of disciplines.

There is also uncertainty in the probabilities of occurrence of scenarios. In this study, we address this uncertainty by identifying important simple scenarios using sensitivity analysis and by examining their effects separately. The procedure is described in the next two paragraphs.

In our scenario analysis, we have combined as many factors as practical into the SYVAC scenarios (Chapter 4). We do this by using a special class of parameters, called switches, to control the selection of mutually exclusive options. For example, the use of a well as a source of water and the use of fresh lake sediment as soil have each been represented as a switch and combined into the SYVAC scenarios. There are four possible combinations for these two switch parameters: well plus lake sediment, well plus no lake sediment, no well plus lake sediment and no well and no lake sediment, each with an appropriate probability of occurrence. Each of these combinations may also be thought of as representing a simple scenario.

We employ switches to combine scenarios because we have developed tools for sensitivity analysis that permit the identification and study of parameters having strong influences on estimated impacts. One such tool is iterated fractional factorial design (Section A.4 in Appendix A), a sensitivity analysis technique that can determine whether any of these switches are important, either separately or in combination with other switches. That is, sensitivity analysis can identify which, if any, of the possible scenarios lead to notably different estimates of impact. We can then examine separately sets of randomly sampled simulations associated with these simple scenarios. This type of analysis is documented in Chapter 6 and in Appendices D and E, where we compare simulations such as those involving the use of the well with those involving use of the lake as the source of drinking water.

It should be noted that a scenario may contain several unique parameters, and that these parameters may be a source of uncertainty. For instance, in cases where the source of drinking water is the well, uncertain parameters include the depth of the well, the amount of water withdrawn by the well (including the amount of water that might be affected by contaminants from the reference disposal vault), and whether the well is also used as a source of irrigation water. In the evaluation of the reference disposal system, we deal with the uncertainty in these parameters through the use of PDFs (Section 2.5.3 and Chapter 5).

2.5.2 Models and Data

Uncertainty in models and data is partly due to our incomplete knowledge of the disposal system. Other uncertainties arise from the constraints we impose on the models, such as the assumption that some model parameters do not vary with time.

For a real disposal vault, many sources of uncertainty will be eliminated or resolved as more information becomes available during successive stages, such as siting (site screening and evaluation), construction, operation and monitoring. Moreover, model estimates for some calculated variables could, in principle, be compared with observations. To minimize these uncertainties, our models and data are founded on the information from an extensive, integrated research program, and we allow for revisions to these models and data following generation of new information. Justification for the models and data used in the current postclosure assessment is discussed in detail in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993).

In many cases, conceptual model uncertainty is included with the use of parameters and their PDFs, because we have developed tools to deal with the effects of parameter uncertainty. We can also use sensitivity analysis to determine whether and how these parameters influence the estimated impacts. For example, in the study of the reference disposal system, the set of groundwater velocities used in the geosphere model (Section 5.4) is based on studies with the MOTIF hydrogeological transport code (Davison et al. 1994b). We include the effects of uncertainties in these velocities with a parameter called the groundwater velocity scaling factor. This factor is described using a PDF with a range of credible values that permits the examination, in SYVAC3-CC3, of groundwater velocities that range in magnitude from 10 times smaller to 10 times larger than the values derived from MOTIF. We also use an adjustable network of segments (Sections 5.4 and 5.5) to describe situations where a bedrock well could perturb flow fields. With this scheme, we can examine the effects of uncertainty in the models and data to determine the degree to which they influence our estimates of impacts.

Where possible in the study, we employ models and data that accurately describe all important processes. Where this is not feasible, we use models and data that would lead to overestimates of impact. An example of the latter case is given by the manner in which we describe the individuals that could be affected by the reference disposal system. In accordance with AECB requirements (AECB 1987a), we assume that the lifestyle of these individuals is based on present human behaviour. However, to ensure that we do not underestimate impacts, we introduce conservative assumptions. For instance, we assume that the individuals spend all their lives near the locations where contaminants might enter the biosphere, and they obtain all of their air, food, water, fuel and building material from sources that would be exposed to these contaminants (Davis et al. 1993).

Finally, we assume that in the study some model parameters take on a constant value over the entire time frame of a simulation or over some finite volume of space. This is the case for the annual precipitation at the disposal site: we assume the value for this parameter is constant in time for each simulation (although the value used will be different from one simulation to the next). We generally invoke this assumption in two cases:

- When the expected dependence on time or space of the parameter is not important. This is the case for annual precipitation: we believe that its variation from year to year is relatively unimportant (Davis et al. 1993).

- When there is insufficient information to model the behaviour of the parameter in time or space. This is the case for processes such as changes to the climate; we have no models currently available that would allow realistic modelling of its effects on the biosphere.

In both of these cases, we choose models and time-independent data that would tend to overestimate impacts. We also examine in separate analyses the effects of disrupting events, such as climate change caused by glaciation (Davis et al. 1993).

Note that, if the time dependence of a parameter in the system model is expected to be important and sufficient information is available to simulate reliably its behaviour, we treat the parameter as a time-dependent variable. This is the case for a variable that describes the container failure rate (Section 5.2.2): its behaviour in time is expressed as a function that depends on several sampled parameters that are time-independent (Johnson et al. 1994b). The system model contains a large number of time-dependent variables, such as the rates of release of contaminants from the used-fuel waste and from the containers, the rates of transport of contaminants through buffer, backfill and rock surrounding the vault, the rates of discharge of contaminants into the surface environment, and the concentrations of contaminants in water and soil used by the critical group.

2.5.3 Probabilistic Analysis

Many model parameters cannot be given precise values for reasons that include imprecise experimental measurement, temporal or spatial variation and an incomplete understanding of all phenomena. One approach to resolve this issue is to use values for all parameters such that the impacts are maximized. However, our experience has shown that it would be difficult to guarantee that a maximum impact has been found: the system model is not simple and impacts may depend on the system parameters in a complicated fashion. More importantly, the resultant impacts would poorly represent the most credible performance of the disposal system and could not be used reliably to find suitable derived constraints or to optimize the safety of the disposal system.

Our approach in the assessment study is focussed on probabilistic analysis to quantify the effect of uncertainty in parameter values. Probabilistic analysis examines the credible range of values for all parameters and produces estimates of effects that reflect the uncertainty in the parameters. Guidelines for choosing the credible range of values for parameters and the relative frequencies of credible values are provided in supporting documents (Stephens et al. 1989, 1993). The distribution of values for each parameter to be sampled have been supplied by experts in the CNFWMP and are fully documented in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993). Szekely et al. (in preparation) describe the PDFs and other data used with SYVAC3-CC3.

In the probabilistic approach, we obtain information on the expected impacts of the reference disposal system by performing many simulations. Each simulation provides one estimate of an impact using one set of values for the input parameters. These values are randomly sampled from the corresponding PDFs. Thousands of simulations such as these, each with a different set of randomly chosen values, provide many estimates of impact. Each simulation can be regarded as a unique "what-if" assessment, and its estimate of impact can be compared with regulatory criteria, standards and guidelines.

Figure 2-3 shows a representative histogram of estimates from a large number of simulations. This histogram captures the uncertainty in the estimates of impact that is due to the uncertainty in the model parameters. (Figure 2-3 uses hypothetical data for illustrative purposes. A histogram of results from the postclosure assessment is shown in Figure 6-17.) The histogram is skewed, and the underlying PDF might be best characterized, in a statistical sense, using a geometric mean and geometric standard deviation.

For the probabilistic analysis, however, the two important statistics are the arithmetic average and arithmetic standard deviation. If the parameter

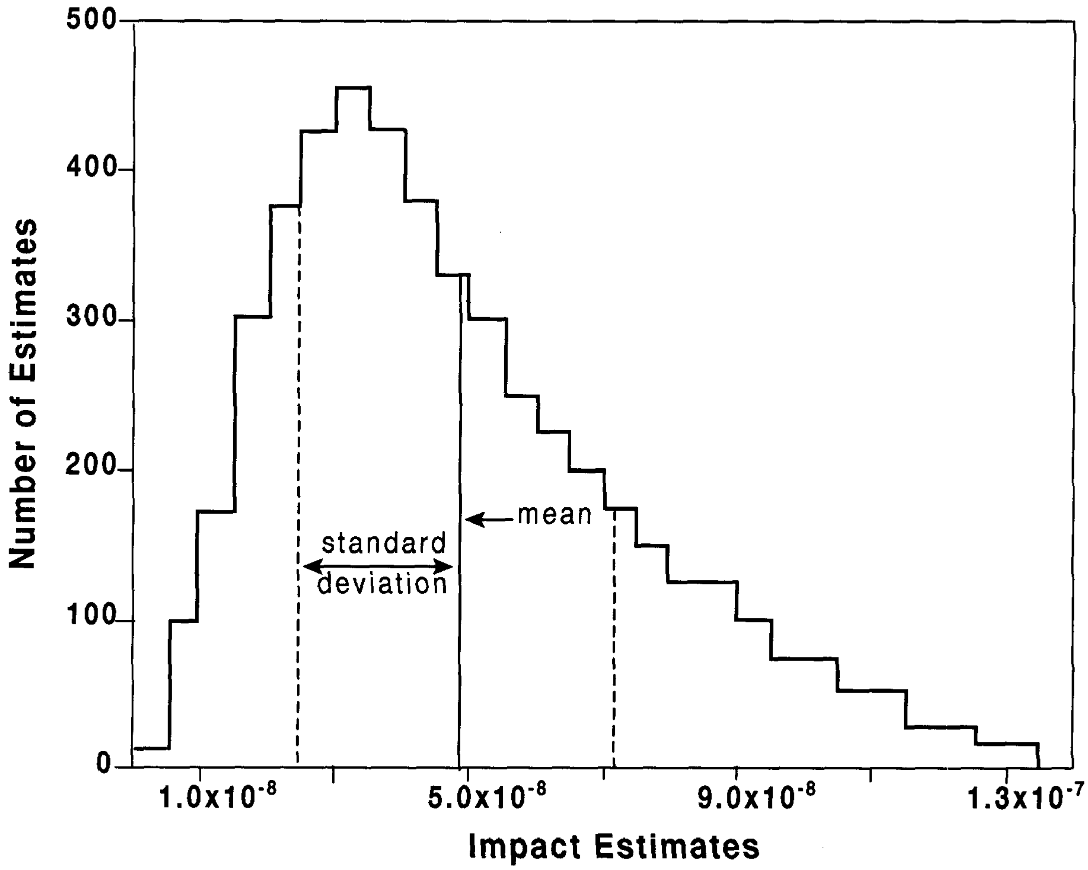

FIGURE 2-3: A Sample Histogram of Hypothetical Impact Estimates

The histogram is representative of results that could be obtained from a large number of simulations carried out using a probabilistic approach. The axis labelled "Impact Estimates" is broken into a set of classes or bins. In the hypothetical results shown, the first bin shows a range from 0 to 0.5×10^{-8} and the last from 1.30×10^{-7} to 1.35×10^{-7} (for radiation doses, the units would typically be sieverts per year). For each bin, the height of the bar is proportional to the number of simulations whose estimated impacts fall within the corresponding range. For example, this figure shows 100 simulations with an impact between 0.5×10^{-8} and 1.0×10^{-8}.

The expectation value of the estimated impact is equal to the arithmetic average, shown here near 4.8×10^{-8}. The width of the histogram is related to the standard deviation (about 2.4×10^{-8} in this example) in the average. Histograms of impact estimates are frequently skewed to the left; that is, bins to the left of the mean generally have larger heights than those to the right. This usually arises because impacts cannot be less than zero, although they often have no upper limit.

values are randomly sampled from their PDFs, then the statistical expectation value of the impact is equal to the average value of the thousands of estimated impacts. That is, the expected impact is the statistical arithmetic average (or mean) of the many estimates of impact. This expected impact can be compared with the regulatory requirements; it offers the advantage (compared with a single deterministic estimate) that it takes into account the specified uncertainty in the model parameters.

A measure of the statistical precision of this expected impact is provided by the standard deviation in the estimated impacts. A smaller standard deviation, or a greater precision in the estimated average impact, can be obtained by increasing the number of randomly sampled simulations. By carrying out a sufficiently large number of simulations with a computer model and its parameter PDFs, we can estimate the average impact computed by the model with as high a statistical precision as we wish. In the results described in Section 6.5, we report results from 40 000 randomly sampled simulations (for the group of radionuclides that contribute most to radiological risk). Our analysis indicates that this number of simulations is sufficient to obtain relatively precise estimates of arithmetic averages.

These arithmetic averages are used to calculate impacts for the reference disposal system. We assert they accurately include the effects of parameter uncertainty because we have specified the PDFs and constituent equations to maximize the coincidence between the estimates and the actual processes expected to occur.

As noted previously, some sources of uncertainty are associated with our imprecise knowledge of the future behaviour of the disposal system and its environment, whereas others are the result of using lumped quantities and their representative PDFs. We have constructed the system model and chosen PDFs so that

- For any particular combination of parameter values, the resulting impact estimate is conservative (for that combination of values) because of the way in which the system model is defined.

- The expected impact, given by the arithmetic average of estimated impacts from thousands of randomly sampled simulations, will be conservative. That is, we believe that our estimate will be greater than the impact that could eventually arise (at the reference disposal system) because of the way in which the system model is defined and the way in which the PDFs are defined.

- The precision of our impact estimate can be calculated from the standard deviation in the thousands of estimated impacts.

2.6 QUALITATIVE ESTIMATES OF IMPACTS

Much of the analysis for the postclosure assessment study is focussed on quantitative estimates of effects. It is not feasible to extend such estimates indefinitely into the future. Factors such as massive changes in the climate could substantially change the characteristics of the disposal system, at a time and in a manner that cannot be quantitatively estimated.

The models and data for the postclosure assessment study of the reference disposal system are designed to yield quantitative estimates of impacts for at least 10^4 a following closure of the disposal facility. They can also be used with caution to estimate trends in effects up to about 10^5 a following closure, providing that a major event, such as a glacial episode, does not occur (or is acceptably represented by the models and data for the reference disposal system). The primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993) give more details on the expected time period of acceptability of the models and data (Section 5.8 provides a summary).

To evaluate the performance of the reference disposal system at long times (beyond 10^4 a), we use the trends to 10^5 a supplemented with reasoned arguments based on well-founded scientific principles and theories. The discussion in Chapter 7 of this report is focussed on specific arguments for the reference disposal system. More general discussion is provided in the EIS (AECL 1994a).

3. DESCRIPTION OF THE REFERENCE DISPOSAL SYSTEM

In this chapter, we outline the features of the hypothetical reference disposal system used in this study (step 1 of Figure 2-1). More specific details are described in Chapters 4 and 5.

3.1 OVERVIEW

In the concept for the disposal of Canada's nuclear fuel waste, the waste would be placed in a vault deep underground in the plutonic rock of the Canadian Shield.

The operating aspects of the disposal facility are described in the primary references describing the engineering design (Simmons and Baumgartner 1994) and the preclosure assessment (Grondin et al. 1994). The features relevant to the postclosure assessment concern the long-term behaviour of the waste in the disposal system, after the rooms would have been filled, the tunnels and shafts would have been sealed, and the surface facilities would have been removed. We assume for the postclosure assessment that short-duration transient effects have ceased. (Our detailed analyses of transient effects such as reflooding (Johnson et al. 1994b) and resaturation (Davison et al. 1994b) indicate it is conservative to assume they are complete at the time of vault closure.) The postclosure assessment then examines the types and magnitudes of possible environmental effects caused by contaminants that might escape from the vault over long times.

One objective of our postclosure assessment study is to demonstrate a flexible assessment approach, applicable to any potential site. The assessment described here is applied to a reference disposal system that is constructed from a reasonably complete set of environmental and geological data, taken largely from the WRA. The results of the assessment apply only to this specific example. However, the method is not otherwise restricted, and we believe it could be applied to postclosure assessments of other disposal systems, including a real nuclear fuel waste disposal facility located at a specific site on the Canadian Shield.

Figure 3-1 illustrates the reference disposal system for nuclear fuel waste disposal evaluated in the postclosure assessment. This reference disposal system includes specific design choices; for example, the vault depth is about 500 m, the thin-walled containers are made of Grade-2 titanium, and the containers are placed in boreholes located in the floor of the vault rooms. The concept for the disposal of Canada's nuclear fuel waste includes other options, such as a nominal vault depth ranging from 500 to 1000 m, the use of different designs and different materials for the containers, and the emplacement of the containers within the vault rooms (AECL 1994a,b).

Other choices assumed for the reference disposal system in the postclosure assessment are outlined below, with other more specific details given in Chapters 4 and 5.

3.2 THE REFERENCE NUCLEAR FUEL WASTE

We assume that the nuclear fuel waste placed in the reference disposal vault consists entirely of used-fuel bundles from CANDU nuclear power reactors. The used-fuel bundles comprise irradiated UO_2 fuel pellets enclosed in Zircaloy fuel sheaths that hold the fuel while it is in the reactor. The bundles contain a large variety of potential contaminants from processes such as fission, radioactive decay and neutron activation. The contaminants of concern for the reference disposal system are listed in Section 5.9; they include both radionuclides and chemically toxic elements.

In the engineering design study reported by Simmons and Baumgartner (1994), it is assumed that the vault holds about 191 000 Mg U. This corresponds to about 100 years of waste at the present rate of accumulation.

For this postclosure assessment study, we initially considered the same mass of fuel in a preliminary analysis. This analysis was aimed at improving the margin of safety of the reference disposal system by identifying, and then imposing suitable constraints on the design of the reference disposal facility. The study (Section 6.2) examined several options affecting the design and layout of the vault. We selected an option with a lesser mass of uranium (1.62×10^8 kg, or 162 000 Mg U) immobilized in about 119 000 disposal containers. This option was chosen to make the best use of the available geological and hydrogeological information from the WRA, and it does not represent a generalized limit for the reference disposal system or for any other potential disposal system.

The identification and selection of design constraints in this preliminary analysis is an example of feedback in the postclosure assessment method.

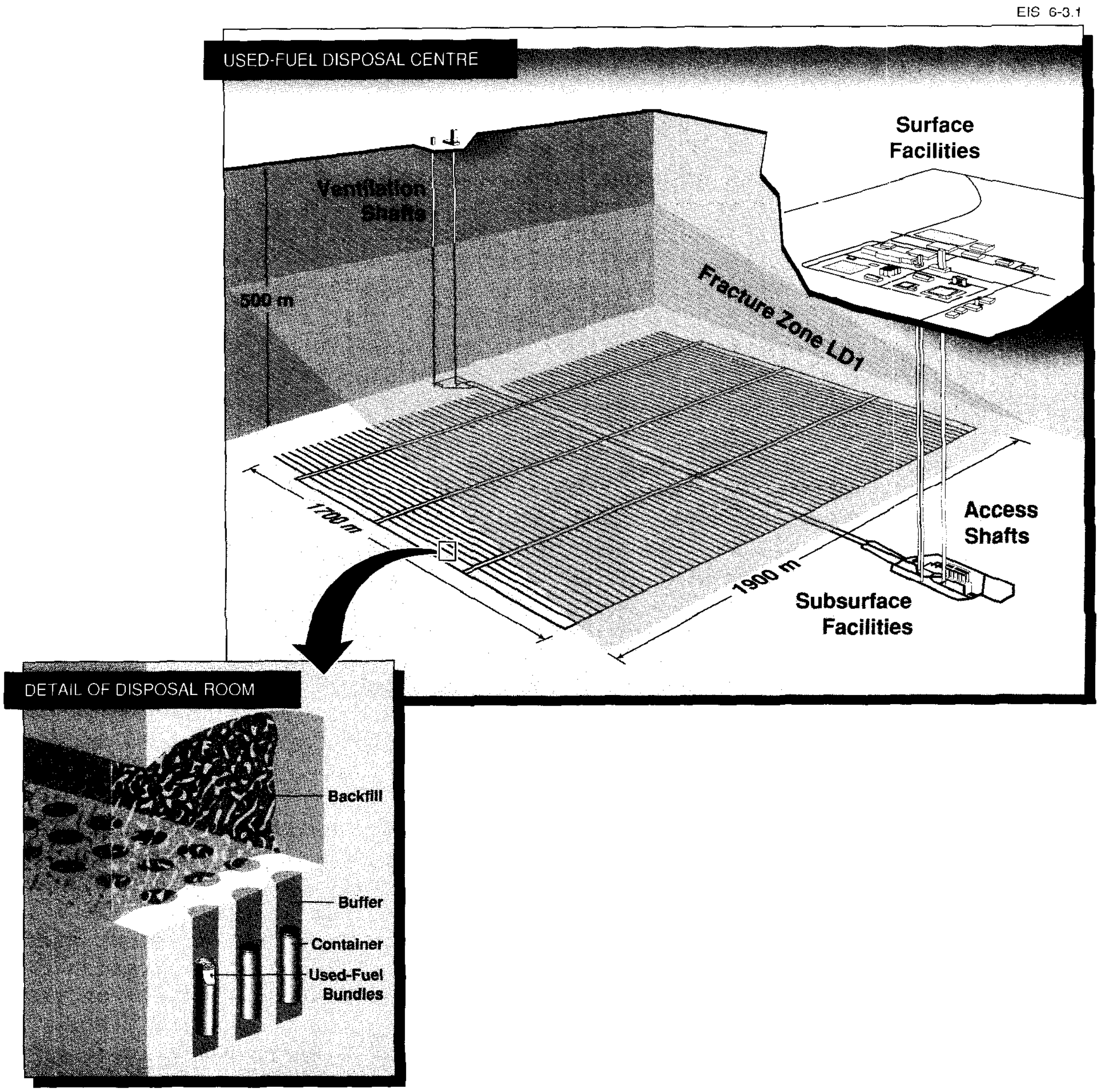

FIGURE 3-1: The Reference Disposal System Evaluated in the Postclosure Assessment

The central feature of the system is a vault constructed in plutonic rock of the Canadian Shield. The vault is about 500 m below the surface and 1900 m long by 1700 m wide. It consists of access tunnels and shafts, with a total of 119 000 containers emplaced in boreholes in the floors of more than 400 disposal rooms. The row of rooms on the right side, near the shafts to the surface facilities, is shorter than the others to separate the containers in those rooms from a fracture zone assumed to pass near the vault. We assume that this fracture zone, known as fracture zone LD1, extends to the overburden near the surface and passes through the plane of the vault. The closest perpendicular distance between the edge of the vault and LD1 is about 50 m.

The inset shows a cross section of a typical disposal room. Used-fuel bundles from CANDU reactors will be placed in corrosion-resistant titanium containers. The containers are located in boreholes in the floor of a disposal room and are surrounded by a dense mixture of bentonite clay and sand (the buffer). Glacial lake clay mixed with crushed rock (the backfill), along with a series of concrete bulkheads, seals the disposal rooms, access tunnels and shafts.

3.3 THE REFERENCE DISPOSAL VAULT

The reference disposal vault used in this postclosure assessment study is illustrated in Figure 3-1. It has been laid out as a rectangle in a horizontal plane at a depth of about 500 m. We assume that a fracture zone, referred to hereafter as fracture zone LD1, extends from the overburden near the surface to below the depth of the vault and cuts through the vault horizon at a shallow angle. The closest distance in a horizontal direction from fracture zone LD1 to a container in any room is about 150 m, and the closest perpendicular distance is about 50 m. That is, a minimum of about 50 m of rock isolates the containers in any vault room from LD1. This rock, at a depth of 500 m and surrounding the disposal vault, has a low permeability and is sparsely fractured (Davison et al. 1994b).

It is unlikely that this particular vault arrangement would be adopted for an actual disposal site. Host rock formations suitable for a disposal vault could contain fractures that require deviations from a completely regular layout. At a real site, mining engineers would design the vault to minimize the effects of nearby fractures; the resulting layout might not be rectangular, nor in a single plane. For the study reported herein, we assume the simple configuration shown in Figure 3-1, with LD1 passing near the vault, so that the effects of such a fracture zone can be evaluated. We also study a special situation where the fracture zone passes through the vault, so that there are rooms above and below LD1. This situation, documented in Section 6.2, is part of the preliminary analyses on derived constraints.

The vault includes access and ventilation shafts, boreholes, tunnels and subsurface facilities. For the postclosure assessment, we assume that all these features have been completely sealed and that they have no influence on the subsequent movement of contaminants. We also assume that there would be negligible effects on groundwater and contaminant movement associated with any damage to the rock that could occur during excavation of the vault (based on detailed studies by Chan and Stanchell (1990) on the low-permeability sparsely fractured rock surrounding the vault.) For assessment of the open-borehole scenarios (Section 6.7), we evaluate a situation in which an open borehole is assumed to pass near the vault from the surface environment.

The vault comprises several hundred disposal rooms that contain the nuclear fuel waste. We assume that the used-fuel bundles are immobilized in corrosion-resistant containers composed of an alloy of titanium. Glass beads in the containers provide mechanical support against external pressures. The containers are placed in boreholes in the floors of the disposal rooms (shown in the inset to Figure 3-1). A layer of a mixture of bentonite clay and sand surrounds the containers on all sides. This layer, called the buffer, is expected to limit the rate of movement of water toward the containers because bentonite has an extremely small permeability. A mixture of glacial lake clay and crushed rock, called the backfill, and concrete bulkheads are used to seal the disposal rooms.

The primary reference describing the engineering design (Simmons and Baumgartner 1994) specifies engineering details such as the spacing of the boreholes in the rooms and the distance between rooms. The main factor controlling this spacing is the release of heat from the used fuel. Nuclear fuel waste is radioactive and gives off heat as the radionuclides decay. In the closed environment of the vault, the containers would at first release heat faster than it could be conducted away by the rock, causing temperature rises in the vault and in the surrounding rock. After about two hundred years, the temperature would reach its maximum, and then start to fall as the net decay rate declines, and heat is released more slowly. Figure 3-2 shows estimated temperatures at the surfaces of containers at different locations in the vault as a function of time. The maximum temperature reached by the containers is less than 100°C, a design limit achieved by adjusting the spacing of the containers and the rooms.

We use the temperature versus time data to estimate processes such as corrosion rates of the containers and precipitation of contaminants in the vault (Johnson et al. 1994b). In making these estimates, we use a simplified geometry to represent the spacing between the boreholes and rooms and the thickness of the buffer separating the containers from the surrounding rock.

Other details on the reference disposal vault are summarized in Sections 5.2 and 5.3. The vault model is fully documented in a primary reference (Johnson et al. 1994b).

3.4 THE REFERENCE GEOSPHERE

We assume that the reference disposal facility for this postclosure assessment study has been constructed in plutonic rock of the Canadian Shield. A study by the Geological Survey of Canada (McCrank et al. 1981) identified over 1000 plutons in central Canada that might be potentially suitable as host sites. To obtain consistent quantitative results in the postclosure assessment, however, we have chosen to characterize the reference disposal system using information from a site where extensive research has been carried out on geological and hydrological features. This site is the WRA, near Lac du Bonnet, Manitoba (Figure 3-3). The WRA and the Underground Research Laboratory have been extensively studied for more than a decade, and a large and consistent set of physical, chemical and geological data and analyses are available (Davison et al. 1994b).

We also assume that fracture zone LD1 passes near the vault, as mentioned above. The locations of other fracture systems in the rock surrounding the hypothetical vault have been identified by remote sensing and from boreholes drilled in the WRA (Davison et al. 1994b). However, excavating the comparatively small URL has revealed much less detail about fractures in the rock than would be found in excavating a real, much larger, disposal vault. Thus the location and characteristics of some fractures have been estimated using expert judgment (Davison et al. 1994b). In addition, we assume that features such as vertical fractures exist in some areas because of the general pattern of these features over the region.

Other details of the rock surrounding the reference disposal vault are summarized in Sections 5.3 to 5.5. The geosphere model is fully documented in a primary reference (Davison et al. 1994b).

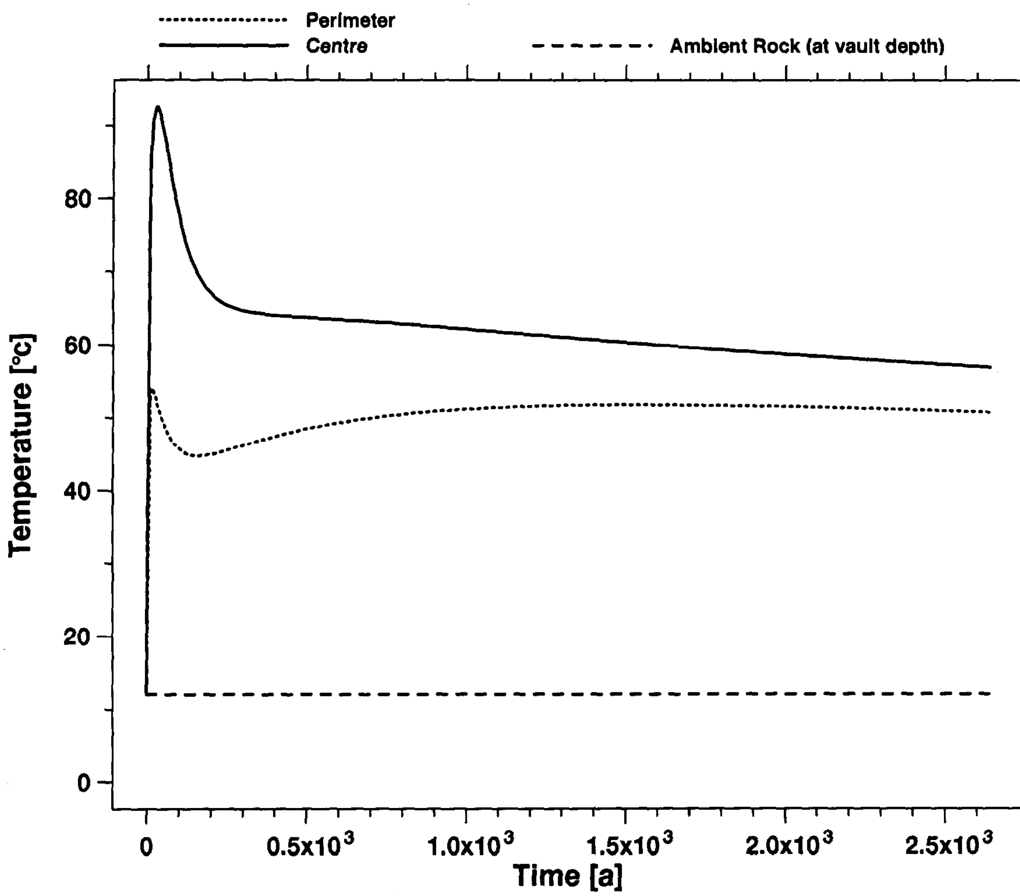

FIGURE 3-2: Vault Temperatures as Functions of Time

The two curves show the estimated temperatures of the surfaces of two containers: one located near the centre and one near the perimeter of the reference disposal vault. The temperature rises because of the release of heat from the radioactive decay of used fuel. The estimated temperatures rise to a maximum of 94°C after about 29 a, near the centre of the vault, but only to 54°C after 13 a, near the perimeter. After about 10^5 a, temperatures in the vault would reach the ambient temperature of about 12°C. (Temperature calculations were made using an analytical code based on a report by Mathers (1985)).

3.5 THE REFERENCE BIOSPHERE

Certain characteristics of the surface environment, or biosphere, at the hypothetical disposal site are also important for the postclosure assessment. Over time, these site characteristics may change from their current state.

EIS 6-3.3

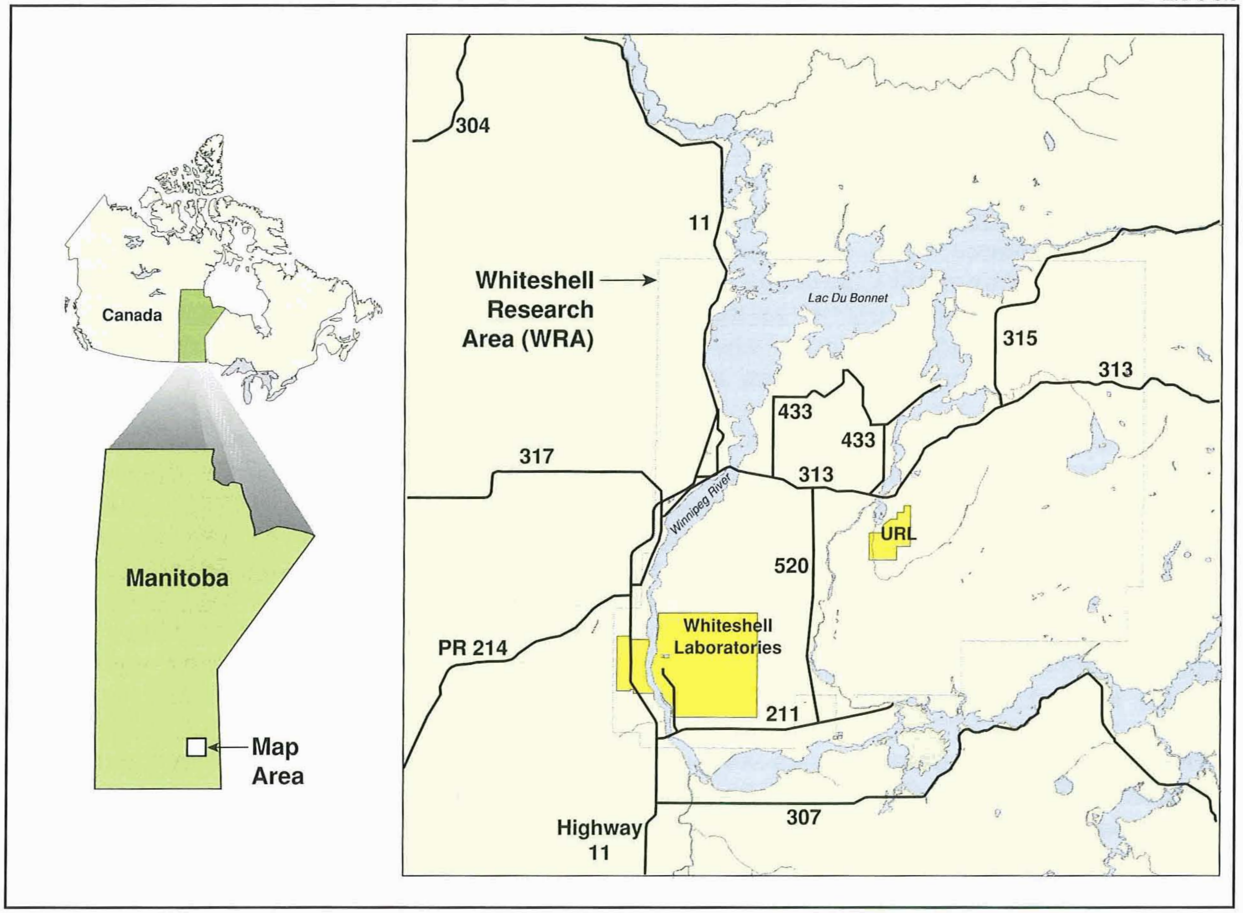

FIGURE 3-3: Map Locating the Whiteshell Research Area

In the postclosure assessment, we constructed the reference geosphere mode by drawing on the extensive set of environmental and geological information available from the Whiteshell Research Area in southeastern Manitoba. This area, which includes the Underground Research Laboratory (URL), has been intensively studied for more than a decade (Davison et al. 1994b).

In the postclosure assessment of the reference disposal system, we assume that site evolution continues according to processes that have operated in the past. Because the Canadian Shield is very old and stable, we assume that no major changes in the topography of the region would occur during the next 10^4 a, the time frame of concern for quantitative estimates of effects.

In the past, continental glaciation has drastically altered the climate on the Canadian Shield and at the WRA. The last great ice cover, over a kilometre thick, melted about nine to ten thousand years ago, and the next major ice age may occur in about 2×10^4 a (Davis et al. 1993). Because this is beyond the 10^4-year time frame of concern, our quantitative estimates of impact do not include the presence of a glacier in the biosphere.

Even so, Davis et al. (1993) have shown that the effects of different glacial states, including states preceding glaciation, would not lead to substantially different estimates of radiation dose insofar as the biosphere is concerned; in fact, different glacial states tend to yield similar estimates of impact. Moreover, Davis et al. (1993) have shown that, although changes in climate, surface water, soils, vegetation, filling of lakes and lifestyle of people will likely occur, changes to the current state would have relatively modest effects on the estimated impacts for times up to about 10^4 a. That is, these changes would have small perturbations on impacts that are estimated if we assume that current (interglacial) conditions will persist over the next 10^4 a. Many of these changes do not require explicit treatment in the biosphere model, whereas some are implicitly included through the use of PDFs used to describe a range of possible conditions (Davis et al. 1993, Davison et al. 1994b).

Finally, we assume that the lifestyle of people living near or on the reference disposal system would be similar to the current range of rural lifestyles that exist on the Canadian Shield (Davis et al. 1993). We believe that such people would receive the largest potential environmental impacts from a disposal vault (Davis et al. 1993, Lawson and Smith 1985), thus corresponding to the critical group concept required by the AECB regulatory guidelines (Section 1.4 and Appendix C). We assume that these people would not be aware of the presence of the vault, thus they would not take action to prevent or mitigate any possible impacts.

Other details pertaining to the surface environment of the reference disposal system are summarized in Sections 5.5 and 5.6. The biosphere model is fully documented in a primary reference (Davis et al. 1993).

4. SUMMARY OF SCENARIO ANALYSIS

In Section 2.1, we noted that our quantitative assessment study is based on a simulation approach, consisting of the six steps shown again in Figure 4-1. In this chapter, we describe the second step, the analysis to identify scenarios for the reference disposal system (Section A.2 in Appendix A; Goodwin et al. 1994). Scenario analysis has been ongoing for more than ten years, and we concentrate here on the final results and conclusions affecting the reference disposal system.

4.1 OVERVIEW OF THE PROCEDURE

Scenario analysis is a systematic procedure with two main objectives. The first is to identify and describe all the possible factors that could influence the ability of the waste disposal system to isolate waste from humans and the natural environment. A factor is a distinguishing characteristic of the disposal system and its surroundings, or a characteristic of perturbing external or internal events. Examples of factors are radioactive decay, characteristics affecting contaminant transport through the buffer, durability of borehole seals, physical properties of the rock surrounding the vault, chemical interactions between contaminants and minerals in the rock, the presence of surface water bodies in the biosphere and human diet.

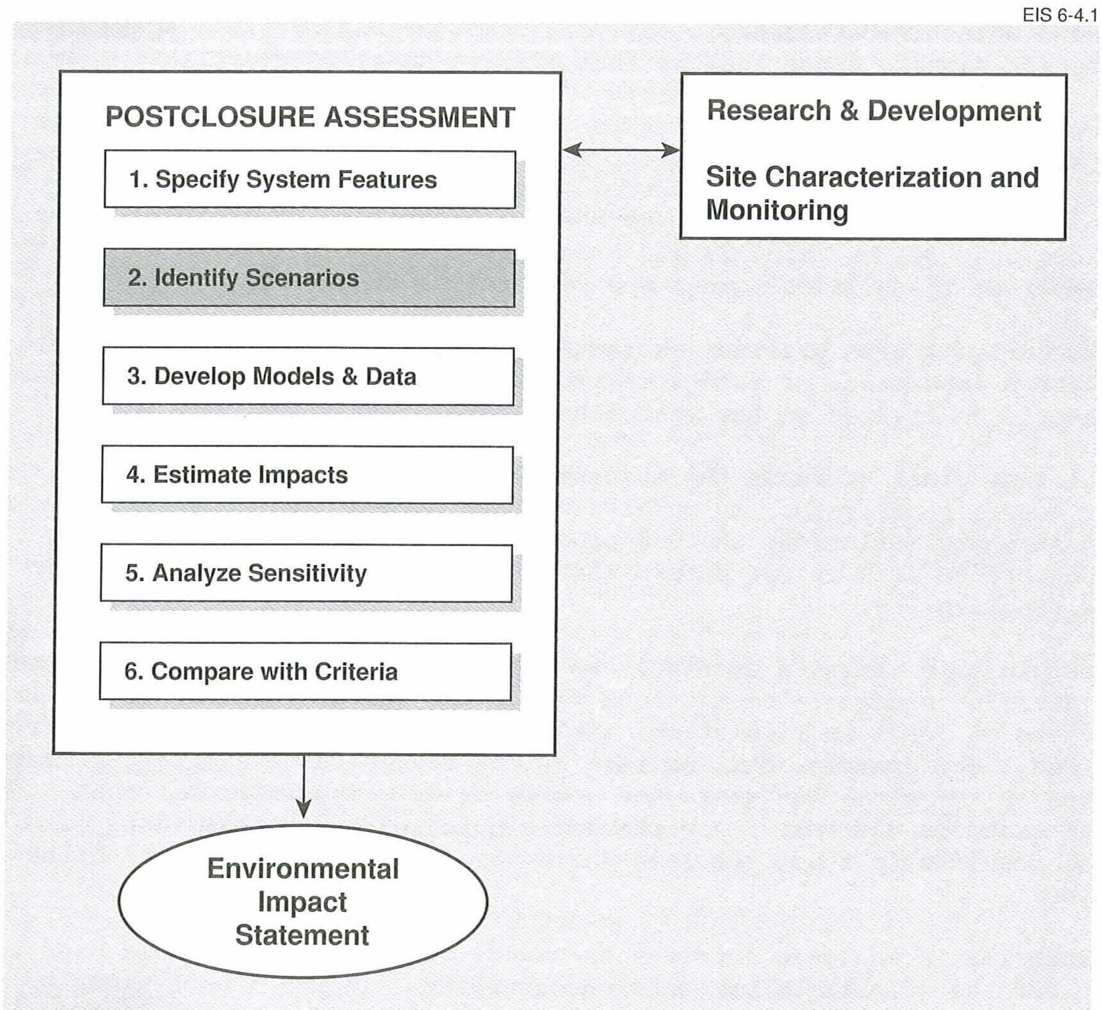

FIGURE 4-1: The Scenario Analysis Step in the Assessment Approach

This figure is similar to Figure 2-1 but highlights the second step, scenario analysis, in the postclosure assessment approach. Scenario analysis is a systematic and comprehensive procedure aimed at identifying all the factors that require further detailed evaluation and determining how these factors should be combined and treated in scenarios. A factor is a distinguishing characteristic of any affected part of the disposal system, such as radioactive decay and contaminant transport through fractures. A scenario defines a possible future of the waste disposal system that includes potential impacts on the critical group or the natural environment.

The specifications of the disposal system (from step 1) define the breadth of scenario analysis. Once scenarios are defined, we proceed to step 3 and develop representative models and data. There is considerable feedback between each of the steps in the postclosure assessment approach. In particular, the probabilistic method used to estimate impacts (step 4), together with the capabilities of the system model (step 3), greatly influence the characteristics of the scenarios that are defined.

The second objective of scenario analysis is to determine, in a consistent and coherent manner, those factors that require detailed quantitative evaluation in the postclosure assessment. The analysis leads us to construct self-consistent combinations (or scenarios) of these factors. A scenario is "a sketch, outline or description of an imagined situation or sequence of events" (NEA 1992). For the postclosure assessment study, a scenario defines a possible future of the waste disposal system and includes a set of factors that define pathways and processes that could lead to an effect on a member of the critical group and the natural environment.

Scenario analysis also provides estimates of the likelihood of occurrence and relative importance of each scenario and recommendations on how a scenario should be treated in the postclosure assessment study.

Feedback from other steps in the assessment approach (Figure 4-1) is crucial to scenario analysis. In particular, the method used to estimate impacts strongly influences the end products of scenario analysis. The influence can be seen in our deterministic and probabilistic analyses of impacts (Section 2.3).

Our deterministic analysis examines the median-value simulation, and we use it for detailed study of interactions within the system model. Because it is focussed on just one simulation, the scope of the deterministic analysis is limited. For example, our analysis of the median-value simulation concentrates on the situation where the source of drinking water for the critical group is the well. A different simulation and further analysis would be required to study the case where the lake is the source of drinking water.

Our probabilistic analysis involves thousands of simulations and is used to account for the effects of parameter uncertainty. It has a much wider potential scope because we can define parameters for the model of the disposal system that effectively define many scenarios. One example is a well-usage parameter, which combines individual scenarios in which either a well or a lake serves as the source of drinking water for the critical group. The probability of occurrence of the well scenario, p_w, defines the probability associated with the use of well water. The lake scenario is assumed to be a mutually exclusive option, and its probability of occurrence is equal to $(1-p_w)$. We then perform a large number of simulations that are sufficient to sample the required mix of simulations that involve the well or the lake as the source of drinking water. This mix of simulations is used in a single analysis to calculate impacts, such as the arithmetic average of annual dose to individuals in the critical group. In addition, sensitivity analysis is used to determine whether the well scenario or the lake scenario, or both, make significant contributions to the annual dose, by examining the sensitivity of the average annual dose to the well usage parameter. Hence rather than analyzing separately the two simpler scenarios involving the use of well water or lake water, we analyze them both in a compound (well plus lake) scenario using a parameter whose values reflect the relative likelihood of these similar but mutually exclusive scenarios.

The flexibility offered by probabilistic analysis means we can simultaneously analyze many scenarios and use our analysis tools more effectively. If we were to use only deterministic analysis to estimate impacts, each scenario would require individual consideration and analysis. The discussion on construction of scenarios (Section 4.1.4) indicates that the number of such scenarios would be very large.

A large group of AECL Research experts contributed to the scenario analysis of the reference disposal system. Their combined expertise included the following disciplines: agronomy, applied mathematics and statistics, biology, chemistry, civil engineering, computer science, ecology, environmental assessment, geochemistry, hydrogeology, limnology, meteorology, mining engineering, nuclear physics, soil chemistry, soil science, structural geology and zoology.

The group used a six-step procedure, shown in Figure 4-2, to identify factors and scenarios and to estimate the relative importance of each scenario for the postclosure assessment study. The following discussion summarizes the procedure and the results of the scenario analysis for the reference disposal system studied in this report. (Section A.2 in Appendix A and Goodwin et al. (1994) provide further documentation.)

4.1.1 Identify Factors

The objective of this step is to identify all the factors that might conceivably have an effect on the behaviour of the disposal system.

The expert group identified over 1000 factors, which were collected into about 300 more broadly defined general factors. For example, a general factor is human diet, which represents many possible food types, such as cultivated and wild fruits, domestic animals, wild game and fish.

4.1.2 Classify Factors

The factors from the first step were systematically classified to look for additional factors not identified in the first step.

Several different classification schemes were used. A few new factors were identified and added to the list.

4.1.3 Screen the Factors

This step involved examining the factors over two time frames: times up to 10^4 a and times beyond 10^4 a. The objective is to identify those factors that require more detailed evaluation in this postclosure assessment of the reference disposal system.

For example, for times up to 10^4 a,

- Factors requiring evaluation are used to construct scenarios (in step 4) for detailed quantitative studies. These studies use mathematical models to simulate the behaviour of contaminants in the entire disposal system and to estimate potential impacts that could occur within 10^4 a (the time frame of concern for quantitative evaluation (AECB 1987a)).

EIS 6-4.2

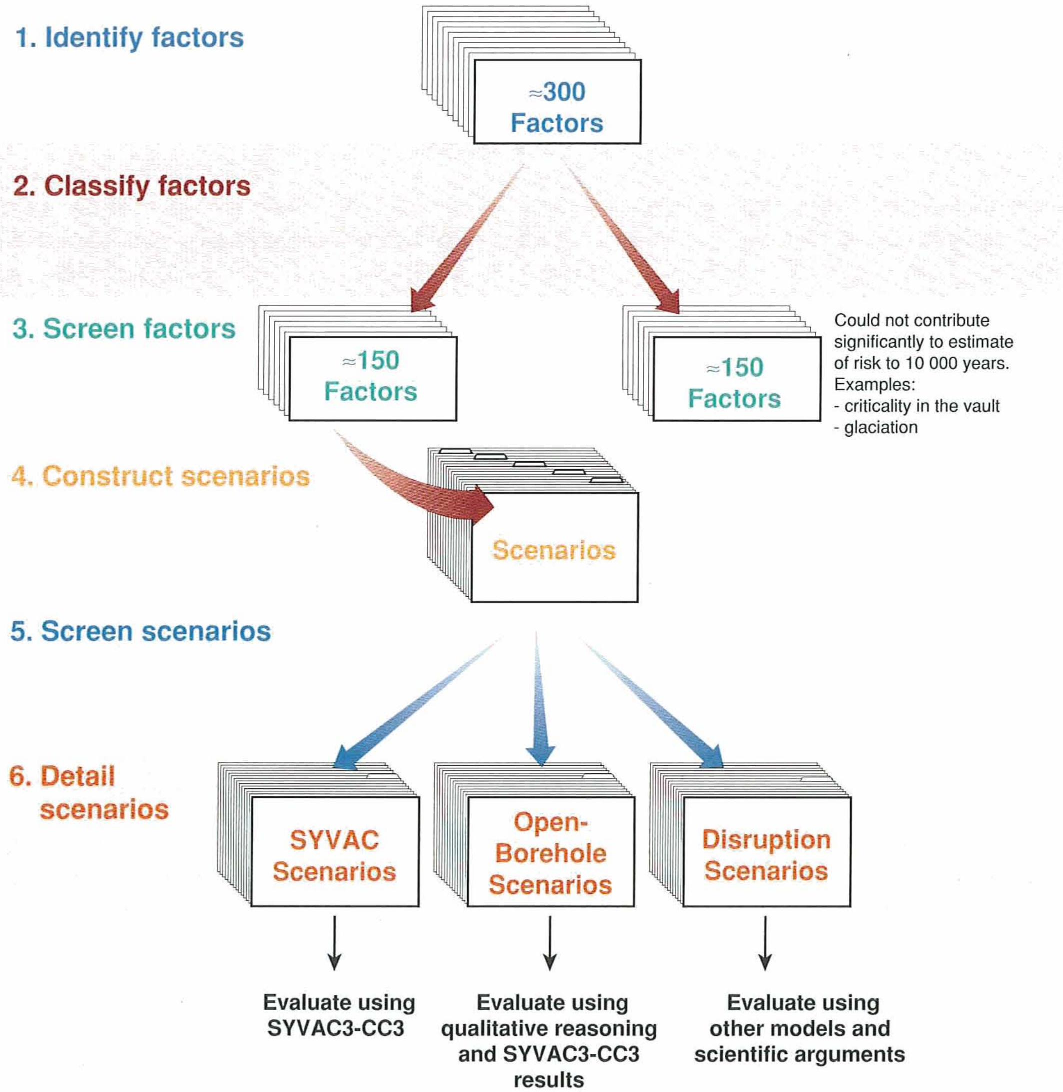

FIGURE 4-2: Summary of Results from Scenario Analysis of the Reference Disposal System to 10^4 a

This figure illustrates the six-step procedure, and results of its application, used to identify factors and define scenarios that require quantitative analysis for times-scales up to 10^4 a. Approximately 300 factors were identified in steps 1 and 2. The screening in step 3 shows that about 150 factors should be considered in constructing scenarios. We believe the remaining factors would have no significant effects on impacts for times up to 10^4 a following closure of the disposal vault (although some may require consideration for times beyond 10^4 a.) Three types of scenarios are constructed in step 4: the SYVAC, open-borehole, and disruption scenarios. All pass the screening in step 5, and thus require quantitative evaluation. In step 6, we more completely define the scenarios and document how they should be evaluated in the postclosure assessment.

- Factors that do not require such evaluation are not included in scenarios for detailed quantitative study because we believe they would not contribute significantly to the estimates of risk. Each of these factors can often be examined on an individual basis without taking into account interactions (or coupling) with other unrelated factors of the disposal system. Frequently it can be shown they could not contribute significantly to estimates of risk from a consideration of their probability of occurrence.

  This is the case, for example, for the potential initiation of a self-sustaining fission reaction (criticality) in the disposal vault. McCamis (1992) has examined this factor and concludes that criticality is not possible; thus no estimates of impacts are required because criticality cannot contribute significantly to estimates of risk.

The expert group decided that about half of the factors do not need to be included in scenarios for detailed quantitative study (Goodwin et al. 1994) because they could not contribute significantly to the estimates of risk within 10^4 a. Some of these factors could be important over longer time frames, and they are consequently taken into account when considering potential impacts for times beyond 10^4 a.

For each of these factors, we provide arguments supporting why they are not included in scenarios for detailed quantitative study. Where possible, the arguments are quantitative; in other cases they are based on expert judgment and opinion. These arguments are outlined by Goodwin et al. (1994), with detailed discussions in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993). Table 4-1 gives some examples of these factors and examples of supporting arguments for their treatment. A factor is often excluded on the basis of the following general arguments.

- The factor falls outside the mandate of the postclosure assessment study of the reference disposal system. On this basis, the group excluded factors that do not apply to nuclear fuel waste from CANDU reactors, to disposal sites in plutonic rock of the Canadian Shield and to titanium-alloy containers. (These factors also do not require evaluation for time-scales beyond 10^4 a.)

- The factor is an event that has an extremely small probability of occurrence. We have taken "extremely small probability of occurrence" to mean one of two possibilities: either we estimate that the annual probability of the event is less than 10^{-8} per year, or we believe that the event would not occur over the next 10^4 a.

  We have made quantitative estimates whenever possible. Sections F.2 and F.3 in Appendix F give examples for two events: meteorite strikes and earthquakes. For other events where we cannot provide a quantitative estimate, we give reasons supporting our opinion that they would not occur: this is the case for criticality and volcanism. Table 4-1 summarizes the reasons and more details are given in the primary references.

TABLE 4-1

EXAMPLES OF FACTORS THAT DID NOT PASS THE SCREENING STEP*

Factor and Description	Comments
Biological Activity. Microorganisms, microbes, bacteria and other biota could change the physical and chemical environment in the vault, affecting corrosion of the containers and other processes. Microbes in the geosphere could affect the movement of contaminants.	Although severely limited by nutrient supply, elevated temperatures and radiation fields, microbial activity is likely to be present in the vault (Stroes-Gascoyne 1989, Stroes-Gascoyne and West 1994). It is expected that the possible effects can be treated through the use of conservative assumptions, such as those used in describing crevice corrosion of titanium containers (Johnson et al. 1994b). In the geosphere, microbial effects are expected to be limited because of the nutrient-poor conditions. Studies at the WRA reveal that only small quantities of microbes and bacteria exist in the groundwaters at disposal vault depths (Davison et al. 1994b). Research on this factor is continuing.
Biological Evolution. Organisms are subject to biological evolution in an everchanging environment, that may affect anatomical features and physiological processes.	It is unlikely that evolution will lead to new and unusual exposure pathways, partly because a wide variety of pathways are explicitly included in the description of the biosphere. These comments also apply to the evolution of humans and other biota. That is, we do not expect that biological evolution will lead to notable changes in estimates of impact because of substantial differences in the characteristics of the biota now explicitly included in the biosphere model.
Chemical Gradients. Movement of salts and contaminants may be enhanced near the waste containers because of temperature changes, ingress of saline water and radiolysis.	It is expected that only radiolysis has the potential to cause significant changes (Johnson et al. 1994b). Radiolysis is included in the SYVAC scenarios through its effects on redox potentials in the vault (and taken into account for times beyond 10^4 a). Salinity and temperature gradients are not expected to have appreciable effects or would not occur to any appreciable extent (Johnson et al.1994b). Thermal buoyancy effects are expected to be unimportant (Davison et al. 1994b).
Climate Change. Changes to the current climate may affect the expected performance of the vault, geosphere and biosphere; for example, changes in average annual precipitation may affect the volume and rate of groundwater in the geosphere. (Glaciation is discussed separately below.)	Elements of this factor are included in the biosphere model; for example, net annual precipitation is described and a wide range of possible values are considered (Davis et al. 1993). It is expected that climate change will not affect the performance of the disposal vault (Heinrich 1984a, Johnson et al. 1994b). Present day groundwater flow conditions in the rocks of the Canadian Shield would not be significantly altered by a climatic change to wetter or drier conditions: the water balance is currently

continued...

TABLE 4-1 (continued)

Factor and Description	Comments
	maintained by only a small influx of the annual precipitation (Davison et al. 1994b). Measurements in the WRA show that the water table remains relatively constant in time, despite large variations in annual precipitation (Thorne 1990). The use of present-day conditions (including topography) will include the effects of a wetter climate, and produce overestimates of impact for a drier climate; warmer or cooler conditions and permafrost would not significantly affect the performance of the geosphere (Davison et al. 1994b). Changes to sea level are not expected to be of concern, because the reference disposal system is hundreds of kilometres distant from the nearest body of sea water. There is a need, however, to consider this factor for times beyond 10^4 a.
Colloids. Changes to the vault environment could promote the formation of colloids, affecting contaminant transport.	Although colloids could form in the containers, studies demonstrate that they cannot migrate through the high-density buffer (Johnson et al. 1994b). Concentrations of naturally occurring colloid-size particles (pseudo-colloids) in granite groundwaters are small, and would have negligible effect on contaminant transport (Vilks et al. 1991a,b; Davison et al. 1994b).
Container Healing. Corrosion holes or pits could heal or close up.	These processes have been omitted, and their omission is expected to lead to overestimates of impact (Johnson et al. 1994b).
Coupled Processes. Coupled processes and irreversible thermodynamics may affect transport of contaminants in the vault.	Analysis of the effect of these processes suggests that they are relatively unimportant compared with diffusion (Johnson et al. 1994b). Processes such as diffusion, corrosion and chemical interactions are included in the SYVAC scenarios.
Criticality. Self-sustaining fission reactions may occur from the accumulation of critical masses of ^{235}U or ^{239}Pu in the vault.	Calculations and analyses suggest that this process is extremely unlikely (McCamis 1992); it would require selective segregation and accumulation of a fissile isotope in relatively high concentration and purity. No possible mechanisms have been identified in the vault environment that would support these requirements (Johnson et al. 1994b).
Earthquakes. Large earthquakes and related events could affect all components of the disposal vault and change the properties of the surrounding rock.	Potential damage includes changes to contaminant release rates from the disposal vault, and new or altered pathways for contaminant movement from the vault to the biosphere. However, these events are thought to have an extremely small probability of occurrence. Probabilities

continued...

TABLE 4-1 (continued)

Factor and Description	Comments
	are less than 10^{-8} per year that an earthquake near the reference disposal system would significantly disrupt the disposal vault, cause movement along an existing fault or cause the formation of a new fault (Section F.3 in Appendix F). Possible effects for times beyond 10^4 a need to be evaluated.
Erosion. Massive erosion of rock could result in important changes to hydraulic heads and contaminant transport.	Merrett and Gillespie (1983) note that rates of rock erosion on the Canadian Shield are about 2×10^{-5} m/a, which is of no concern for a deep underground vault. Studies of glacial erosion of rock in eastern Canada (Kaszycki and Shilts 1980) show that the depth of erosion ranges from only 2 to 10 m per glacial event.
Formation of Gases. Chemical reactions may produce gases, such as hydrogen, which could affect contaminant movement in the vault.	The vault design for the reference system excludes carbon steel, a primary source of hydrogen. Screening calculations have shown that hydrogen produced by radiolysis and corrosion of Zircaloy and titanium would not lead to formation of a gas phase within 10^4 a (Johnson et al. 1994b). Generation of other gases (such as methane) requires further research and evaluation. This factor needs to be considered for times beyond 10^4 a.
Geochemical Evolution of the Buffer, Backfill and Rock. Hydrothermal alteration and other geochemical processes could lead to alteration of the properties of the buffer, backfill and rock near the vault.	Vault temperature will be less than 100°C (Baumgartner 1993), and no large concentrations of unusual and reactive chemicals are expected in the vault. Under these conditions, chemical and physical changes are expected to be slow (Johnson et al. 1994b). For example, conversion of the buffer clay (bentonite) to a nonswelling clay (such as illite) would not occur to any appreciable extent in 10^4 a (Johnson et al. 1994b). Possible effects for times beyond 10^4 a need to be considered.
Glaciation. Glaciation will change stress fields, flow regimes and temperatures, and could have many complex effects on the vault, geosphere and biosphere.	It is not likely that the next glacial episode will occur before about 2×10^4 a from now (Eronen and Olander 1990, Davis et al. 1993). This is beyond the time period specified by the AECB (1987a) for quantitative evaluation. Glaciation will have a mixed influence on the disposal system: it will have massive effects on the biosphere, but it would not affect the performance of the vault (Heinrich 1984a). Davis et al. (1993) examine the effects of glaciation in some detail, and conclude that the biosphere model, designed to simulate current interglacial conditions, is likely to overestimate impacts compared with other possible glacial states.

continued...

TABLE 4-1 (continued)

Factor and Description	Comments
	The possible effects of glaciation for times beyond 10^4 a need to be considered.
Meteorites. A large meteorite striking near the disposal vault could significantly disrupt all engineered and natural barriers, and lead to significant radiation doses and risk.	Although large radiation doses and other environmental impacts are possible, the probability of occurrence of this event is extremely small. We document in Section F.2 in Appendix F an estimate for the case where a large meteorite creates a crater that moves and redistributes rock to a depth of 500 m (the nominal minimum depth of the disposal vault). The estimated probability of occurrence is extremely small, approximately 10^{-11} per year. Effects over longer time-scales should be considered.
Monitoring and Remedial Activities. Boreholes to monitor performance could provide pathways for contaminant transport.	In the concept for the disposal of Canada's nuclear fuel waste, it is intended that monitoring would not be an essential technical requirement for the postclosure phase. Nevertheless, monitoring may occur. We assume that monitoring and all such activities would be closely constrained so that the safety of the disposal system would not be compromised.
Radiation Damage. Radiation fields could damage the vault and surrounding rock.	Experimental evidence shows that gamma radiation will have little or no effect on the crystal structure of the buffer (Oscarson and Cheung 1983). No damage to the rock surrounding the vault is expected.
Rock Properties—Undetected Features. Features such as unknown active fracture zones may have significant effects on groundwater flow and contaminant transport.	It will take several decades to select, operate, close and decommission an actual disposal facility and, during this time, underground characterization studies will be continued. It is reasonable to expect that, by the time the decision is taken to close the vault, all features that could have any significant effects will have been detected, and that a suitable model of the host rock will have been prepared. The models used with the SYVAC scenarios for the disposal system studied in this assessment contain all properties known to be important. It also includes features (with pessimistic properties) that are introduced to study their effects on safety, such as a fracture zone extended to pass through the horizon of the vault.
Shaft and Borehole Seal Failure Failure of the shaft or borehole seals could modify groundwater flow and contaminant transport.	Elements of this factor are included in the vault and geosphere models, mostly through the uncertainty specified for key parameters. However, no important changes in groundwater flow (and subsequent contaminant transport)

continued...

TABLE 4-1 (concluded)

Factor and Description	Comments
	are expected because the vault design includes a redundant combination of bulkheads, seals and backfill in the shafts and boreholes that would control and limit groundwater movement for long periods of time (Johnson et al. 1994b). In addition, the shafts would be remotely located from any vault room containing used-fuel waste (typically 100 m or more), thus further reducing any possible effects on the movement of contaminants in the geosphere. Most boreholes would also be located far from any vault room containing waste (see also the discussion in Section 6.7).
Urbanization on the Discharge Site.	Although the discharge site could become urbanized, it is reasonable to expect that overestimates of impact would always be obtained by assuming the discharge site is rural (Davis et al. 1993). A rural group of people tends to be more self-sufficient than an urban group, and they would tend to rely more on local water, food and other resources. These resources would likely be more contaminated if obtained from the vicinity of the discharge area. Because impacts are estimated for the group at most risk (the critical group), it is conservative to assume that they have the characteristics of a rural group and that the discharge site is rural. Urban ecosystems tend to be very limited compared with rural ones, thus assuming a rural setting is also conservative for assessing environmental impacts.
Volcanism. Volcanism (hot spots and rifts) and magmatic activity could cause activation of faults, changes in topography, changes in rock stress, deformation of rock, and changes in groundwater temperature and composition.	These processes are very unlikely for plutonic rock of the Canadian Shield. There are no hot spots on the Shield at present, and no evidence that plate tectonics would move the Shield over any hot spots within the next 10^4 a (Davison et al. 1994b). The site selection process would also exclude regions where such activities are of potential concern (Davison et al. 1994a). This factor should also be examined for time-scales beyond 10^4 a.

* This table lists some of the factors that are not included in the construction of scenarios requiring detailed quantitative evaluation for times up to 10^4 a. Taking into consideration their potential importance, we concluded they would not contribute significantly to estimates of risk within 10^4 a. A brief comment supporting this decision is given in the table; more details are provided in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993). The comments also indicate whether the factor is taken into account for times beyond 10^4 a.

- The factor is a process that would not occur to any appreciable extent over the next 10^4 a. This consideration supports the exclusion of factors such as (geological) metamorphic activity and extremely slow geochemical processes. We have also eliminated glaciation because the next onset of a major glacial episode is not expected before about 2 x 10^4 a from the present (Davis et al. 1993). (If glaciation did occur before 10^4 a, it is unlikely that the critical group would reside near the zones of potential contaminant discharge. Even if their place of residence did not change, their food and energy requirements would likely be obtained from areas outside of the discharge zones. Thus it is reasonable to expect that impacts would be larger if it is assumed glaciation does not occur.) Separate studies have been carried out on how a glacial episode could affect the biosphere (Elson and Webber 1991, Davis et al. 1993) and the geosphere (Davison et al. 1994b). No effects on the vault are expected (Heinrich 1984a, Johnson et al. 1994b).

Some of the factors in Table 4-1 may require consideration for their potential effects at times beyond 10^4 years and are evaluated further in the EIS (AECL 1994a) and in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis 1993).

Table 4-2 lists some of the factors that passed the screening in step 3 for times up to 10^4 a, with a brief description of why the factor is expected to be important: they require further quantitative evaluation and estimates of impact in one or more scenarios for times up to 10^4 a. All these factors are also considered in the qualitative evaluation of impacts for times beyond 10^4 a.

The primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993) discuss these factors in greater depth.

4.1.4 Construct Scenarios

The factors from step 3 were organized into three types or groups of scenarios.

- The first type contains most of the factors from step 3, integrated into a system model. In these scenarios, the primary pathway leading to impacts involves normal or expected groundwater-mediated processes, in which waste materials are released from the vault, traverse the geosphere, enter the biosphere and potentially cause radiation doses to members of the critical group and other biota (and to other environmental impacts). The system model, described in Chapter 5, is contained within the computer code SYVAC3-CC3; hence we refer to this group of scenarios as the SYVAC scenarios. (Interim studies and the primary reference for the biosphere model (Davis et al. 1993) use the term "central group of scenarios.")

TABLE 4-2

EXAMPLES OF FACTORS USED TO CONSTRUCT SCENARIOS*

Factor and Description	Comments
Animal Soil Ingestion	Terrestrial animals routinely ingest soil inadvertently or sometimes purposefully to meet nutritional needs (Zach and Mayoh 1984). Soil may be ingested directly or through contaminated plants. Soil from natural salt licks formed by discharge of deep groundwater is particularly attractive to some animals.
Backfill and Buffer Characteristics	The movement of water and contaminants will be affected by properties such as porosity, tortuosity, hydraulic conductivity, temperature gradients, swelling pressure and sorption.
Bioaccumulation, Bioconcentration and Biomagnification	Contaminants may concentrate and accumulate in different organisms, including members of the critical group. Bioconcentration refers to the ability of an organism to concentrate a contaminant from its environment, usually from water or soil; bioaccumulation refers to the tendency of an organism to continue to bioconcentrate throughout its lifetime; biomagnification refers to the occurrence of a contaminant at successively larger concentrations with increasing trophic level in the food web (Zach and Sheppard 1992).
Boundary Conditions	Processes occurring at the boundaries or interfaces between the waste form, container, buffer, backfill and rock may be important.
Climate (biosphere)	A wide variety of climatic factors, such as temperature, precipitation and wind speed, can influence the behaviour and transport of radionuclides in the environment. For example, temperature influences heating fuel needs, which in turn may influence radionuclide concentrations in indoor air and the inhalation dose to humans. Climate is an important driving force for contaminant transport through the soil (Sheppard 1992) and the atmosphere (Amiro 1992b).
Container Failure	Containers could fail before their design lifetime, because of welding or material defects, mishandling and breakage during transport. Long-term container failure could be affected by factors that include elemental solubilities, thermal transients (duration and temperature rise) and the presence and concentration of reactants (such as chloride, sulphide, acids and oxidants).

continued...

TABLE 4-2 (continued)

Factor and Description	Comments
	Possible failure mechanisms include delayed hydride cracking, pitting and uniform corrosion.
Convection, Dispersion and Diffusion	Contaminant transport may occur within the buffer, backfill, rock and biosphere by these processes. Convection and dispersion involve transport in moving water and air; dispersion is caused by variations in velocity and path lengths and acts parallel to and transverse to the direction of convection. Diffusion occurs from regions of high-to-low chemical potential, and also acts parallel to and transverse to the direction of convection. (Matrix diffusion generally refers to the diffusion of contaminants in the transverse direction only.) Dispersion is a fundamental aspect of contaminant transport in the surface environment where it refers to the movement of a contaminant away from its source and its dispersal in soil, water and air through a variety of processes.
Correlation	Model parameters are not always independent; that is, given a value for one parameter, the value for another may be restrained or fixed. Examples include different chemical elements that may show some degree of correlation in solubility limits in the buffer; two segments of adjacent rock may have a similar suite of minerals and subsequently similar sorption properties and conductivities; and the amount of water a person drinks may be related to the amount of food consumed.
Discharge Zones	Groundwater discharge may occur to surface water bodies (rivers, lakes), to a well, to unsaturated terrestrial soils, and to wetlands.
Fires	Fires are routinely used to clear land for agricultural use, to reduce peat, to kill weeds and to remove stubble. Forest fires are an important natural feature on the Canadian Shield, occurring fairly frequently (Amiro 1992b). The material being burned could be contaminated and, upon burning, could inject contaminants into the air as gases or particulates.
Formation of Cracks in Rock	Cracks and faults could form or exist within or near the vault, affecting the performance of seals, grouts and the buffer. Cracks may form due to failed seals, excavation damage to the surrounding rock, faulty buffer materials, and voids in the buffer and backfill.

continued...

TABLE 4-2 (continued)

Factor and Description	Comments
Groundshine	When outdoors, humans and other organisms may be externally exposed to a variety of radiation sources. These may include contaminated vegetation, animals, rocks, and buildings, but chief among them is the ground. Ground exposure, or groundshine, can be an important source of radiation.
Human Diet	The diet of humans can vary greatly, both in type and quantity. Food types include cultivated and wild fruit, domestic animals, wild game, fish, mushrooms etc. Water is also an essential component of diet.
Human Intrusion	Human intrusion could occur for reasons that include retrieval of used fuel, mineral exploration and construction of water wells. Intrusion to retrieve useful material is unlikely because of the expected cost and effort; if it did occur, it is reasonable to assume that those responsible would possess the technology to deal with the hazards. Mineral exploration cannot be ruled out, even though it is unlikely because site selection will favour a host rock that is of little or no known economic value (Davison et al. 1994a). Finally, human intrusion involving the use of a well for drinking water and for irrigation might be important.
Human Soil Ingestion	Humans may ingest soil with food or from their hands (Hawley 1985). This can lead to the ingestion of contaminants in the soil.
Inventory	The waste disposal system should include consideration of all potential sources of radiotoxicity and chemical toxicity. The major sources are expected to be the used UO_2 fuel and its Zircaloy sheaths.
Irrigation	Watering of gardens is common practice on the Canadian Shield. Irrigation water from surface water or wells could be contaminated, and in turn could contaminate plants through root uptake or leaf deposition.
Lake Infilling	Lakes on the Canadian Shield may gradually fill in and be transformed into wetlands and eventually dry land with rich soils suitable for agriculture. Lakes may also be drained and their sediments used for farming. Alternatively, sediments might be dredged to enrich poor soils. In all these cases, soils could be contaminated from sediments. This could be important because sediments

continued...

TABLE 4-2 (continued)

Factor and Description	Comments
	may become contaminated from below, through discharges from the geosphere, and from above, through deposition from the water column.
Open Boreholes	Boreholes inadvertently left open at the time of vault closure could modify groundwater flow and contaminant transport, including transport within the borehole and within the rock surrounding the borehole. This factor is thought to be unlikely because the engineering designs for the disposal facility call for the permanent sealing of all boreholes, including those drilled during site characterization and during facility operation. Screening studies suggest that the situation with the greatest risk is where an open borehole has been drilled from the surface and passes close to a vault room that contains nuclear fuel waste.
Precipitation and Dissolution	Solubility constraints may be important in controlling transport in the buffer, backfill and container. The dissolution rate of the waste matrices could be affected by local dissolution and precipitation; these processes are a function of temperature and other variables.
Radioactive Decay	Radioactive decay, including the ingrowth of progeny, will affect the movement and concentrations of contaminants. Members of a radioactive decay chain may have different sorption and transport properties, which would lead to differences in their transport.
Radiolysis	Radiolysis is the dissociation of molecules caused by the absorption of high-energy radiation. It may change the chemical environment in the vault, locally affecting the electrochemical potential and concentration of reactive radicals.
Rock Properties	Important features of the rock related to contaminant transport include porosity, tortuosity, permeability, active (or open) fracture joints or zones, inhomogeneities and structures such as layers or zones of different rock. It should also be recognized that rock properties such as permeability measured in the laboratory may be significantly different from in situ values.
Sediments	Contaminants may adhere to various particles suspended in the water column and settle to the bottom, and later become resuspended. The deeper, compact sediments may be contaminated from below, by contaminated groundwater discharging from the geosphere.

continued...

TABLE 4-2 (continued)

Factor and Description	Comments
Soil	Soil is the basis of terrestrial food webs because it is required by plants that carry out photosynthesis. Soil is also important in recycling of materials through the action of various invertebrates and microbes. When soil becomes contaminated, a variety of exposure pathways are opened up, most notably root uptake. Important factors related to contaminant transport include soil depth (and the different soil layers), leaching, capillary rise, pore water pH and soil type.
Sorption	Sorption is a collective term used to describe the partitioning of contaminants in groundwater onto surrounding substrates. It is an important process in the buffer, backfill, rock, lake sediment, overburden and soil, and may result in substantial delays in contaminant transport. Sorption depends on factors such as characteristics of the contaminant, substrate and water (such as contaminant concentration, substrate surface area and and groundwater salinity). Sorption on soils is important because sorbed contaminants cannot be taken up by plants or leach or move upward by capillary rise.
Stability of UO_2	The thermodynamic stability and solubility of UO_2 could be affected by a number of variables, such as electrochemical (redox) potential, pH, solutions containing significant concentrations of calcium or sodium ions and availability of organic complexing materials.
Surface Water Bodies	It is likely that contaminants released from an underground vault would first enter the biosphere through discharge of deep groundwater into a lake or river. The fate, as well as the environmental and human impact of the contaminants, would then depend to a large extent on the physical, chemical and biological attributes of the surface water body. Important attributes include size, flushing rate, pH, sedimentation rate and productivity. Various exposure pathways, such as transfer to fish, ingestion of drinking water and water immersion, relate to surface water bodies.
Temperature Effects in the Vault	The heat released by the containers will increase the temperatures in the vault. These higher temperatures will affect chemical reactions in the vault, such as container corrosion and transport of contaminants by diffusion.

continued...

TABLE 4-2 (concluded)

Factor and Description	Comments
Topography	Topographical features of the earth's surface relevant to contaminant transport include outcrops and hills, surface water bodies, wetlands, recharge areas and discharge areas.
Uncertainties	The waste disposal system consists of many components that could have complex physical, chemical and biological interactions. Considerable uncertainties exist in modelling its behaviour over 10^4 a; virtually all of the factors that could affect long-term safety have associated uncertainties that must be taken into account.
Water Source	Potential water sources for humans, such as lakes, rivers and wells, could be contaminated to different degrees, and thus impacts would depend on the exact water source. This is particularly true for drinking water of humans and farm animals.
Wells	One or more wells drilled to supply domestic or irrigation water may intersect the contaminant plume. They include high-demand wells that withdraw sufficiently large volumes of water so as to substantially perturb existing deep groundwater flow patterns.

* This table lists some of the factors that require detailed quantitative evaluation in the postclosure assessment for times up to 10^4 a, based on consideration of their potential to influence the ability of the disposal system to isolate waste or to produce a safety or environmental impact. Their influences are discussed in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993). Most of these factors are included in the SYVAC scenarios. The remainder are dealt with in the open-borehole and human intrusion scenarios.

- The second type of scenarios is referred to as the open-borehole scenarios (also called the alternative scenario in the primary reference for the biosphere model (Davis et al. 1993)). They contain the same factors as those in the SYVAC scenarios, with the addition of a factor identified as "open boreholes" in Table 4-2. This additional factor describes an unlikely situation in which we assume an unsealed borehole passes near the disposal vault from the surface environment. We expect that such a borehole could cause significant (but localized) perturbations to existing groundwater flow patterns. Moreover, an open borehole could become an important pathway for the transport of contaminants from the disposal vault.

- The third type of scenarios, referred to as the disruption scenarios, accounts for unlikely events that could significantly affect the integrity of the reference disposal system if they occurred in the vicinity of the disposal vault. At the completion of our analysis, we had identified only one such disruptive event: inadvertent human intrusion caused by a drilling operation. Its probability of occurrence is very small, so that only one such event needs to be evaluated.

In constructing these scenarios, we were guided by several considerations.

During the development of models and associated data (step 3 of Figure 4-1), we found it possible to include more and more factors in the SYVAC scenarios. In fact, we were able to include all but two of the factors in the SYVAC scenarios (and the SYVAC3-CC3 system model). This achievement is important because it permits more efficient use of our analytical tools for systems variability analysis and sensitivity analysis.

While many important factors could be included in the SYVAC3-CC3 system model, we concluded that some factors would require a different approach. This is the case for the unique factors defining the open-borehole scenarios and the disruption scenarios.

For the open-borehole scenarios, our analyses (Section 6.7) make use of reasoned arguments supported by the interpretation of results from SYVAC3-CC3 to evaluate potential impacts.

Evaluations of the disruption scenarios are also performed separately from the SYVAC scenarios. We find it is more practical to evaluate a low-probability scenario using a separate system model that is focussed on estimating impacts for the corresponding factor. Although the SYVAC scenarios can include a low-probability factor, estimating the impacts of the factor becomes inefficient when its probability is very small. For instance, if the SYVAC scenarios included a factor whose probability of occurrence is 10^{-5}, then we would need to perform about 4×10^5 randomly sampled simulations to be confident (at the 95% level) that the factor would have been sampled at least once (Andres 1986) and that its impact has been taken into account.

As noted earlier, the SYVAC scenarios can be regarded as a collection of many scenarios. This is made possible because of the flexibility offered by the systems variability approach and the computer code SYVAC3-CC3 (Section 2.3). Input parameters used by SYVAC3-CC3 are characterized using PDFs to account for uncertainty. SYVAC3-CC3 also permits the use of parameters called switches to control the selection of mutually exclusive options. Switches describe different choices from a finite set of possibilities or scenarios; they are generally characterized using piecewise uniform PDFs (Figure A-6 of Section A.3 in Appendix A) to represent the probability of occurrence of different choices.

Through the use of these switches, we have included many different sets of possibilities (or many scenarios) in the system model represented by SYVAC3-CC3. Thus SYVAC3-CC3 contains many different scenarios, which we refer to collectively as the SYVAC scenarios. We use switches in SYVAC3-CC3 to control choices (selection of scenarios), such as

- whether the critical group's source of drinking water is a well or a lake;
- whether the critical group uses lake sediments as soil for the garden;
- whether the critical group's garden is irrigated (and whether the water is from the well or the lake);
- whether the forage field used by domestic and wild animals is irrigated;
- whether the critical group's household is relatively large or small;
- whether the critical group uses wood or peat as a source of household heat;
- whether the critical group uses organic or inorganic building materials;
- whether the fields used by the critical group have clay, loam, organic or sandy soil; and
- whether (and to what extent) the rate of water withdrawal from a well affects groundwater flow pathways and hydraulic heads at depth in the rock of the geosphere.

We have assumed these choices are mutually exclusive. For example, we assume either a lake or a well serves as the source of drinking water for an individual, although in reality both may be used at the same time or at different times over the lifetime of the individual. Because they are mutually exclusive, our analysis will examine the extreme cases, an important aspect of any assessment. Moreover, we can also weight the estimates of impact from the extreme cases to examine intermediate cases, if it is suspected that an intermediate case yields larger impacts.

Figure 4-3 illustrates how four of the switches used in SYVAC3-CC3 cover 32 scenarios.

We can also identify many other scenarios in SYVAC3-CC3 that are not explicitly associated with switch parameters. For example, we could define scenarios such as

- *The "overburden-well" scenario*. One parameter used to characterize the well is its depth. We define the overburden-well scenario to cover those situations in which the well is relatively shallow and is confined to the overburden. The bedrock-well scenario would describe situations in which the wells extend into the bedrock.

- *The "high-demand well" scenario*. The volume of water withdrawn from the well is calculated from a number of parameters, such as size of the critical group and whether the well is used for both drinking water and irrigation. We define the high-demand well scenario to cover situations where the volume of water withdrawn is large enough to perturb substantially existing groundwater flow patterns. For a well located in the WRA, such perturbations would occur for well demands of the order of 10^4 m^3/a (Reid and Chan 1988, Reid et al. 1989, Davison et al. 1994b).

- *The "early container failure" scenario*. Several parameters are used to describe the rate of failure of containers, and combinations of values may be used to define situations where there is a larger-than-average failure rate attributed to initial fabrication defects. Another combination of values may be used to define situations in which the primary failure mechanism is crevice corrosion.

- *The "large groundwater velocity" scenario*. Uncertainties in groundwater velocities throughout the geosphere are described using a groundwater velocity scaling factor (Section 5.4) whose PDF range covers several orders of magnitude. We may define a large groundwater velocity scenario to correspond to those situations where velocities are greater than average.

The number of possible scenarios can quickly rise to an unmanageable number when all the switch and other parameters (such as the depth of the well) are considered one by one; for example, the 32 scenarios in Figure 4-3 are due to only four switch parameters. However, all of these scenarios are included in SYVAC3-CC3. Thus all can be evaluated together to give integrated estimates of impact. In addition, sensitivity analyses of SYVAC3-CC3 will identify which of these scenarios yield larger estimates of impact.

To evaluate all of the scenarios in SYVAC3-CC3, we follow a probabilistic approach (Section 2.3), in which we analyze thousands of randomly sampled simulations. That is, for each simulation, we randomly select a value for every parameter from its PDF. This random sampling includes all switches, and thus we will select the intended mix of scenarios. For example, if the probability of occurrence of the well scenario is 0.5, then it is reflected in the PDF for the well-usage parameter, and we sample this scenario (about) 500 times in 1000 simulations and 20 000 times in 40 000 simulations. The risk associated with the SYVAC scenarios is proportional to the arithmetic average of the annual dose estimates (ADE) from the thousands of randomly sampled simulations (Section 1.4 and Appendix C). Thus our calculation of average annual dose and risk involves the appropriate number of simulations in which a well serves as the source of drinking water for the critical group. In addition, our sensitivity analyses (Section A.4 in Appendix A) will identify whether the use of the well is an important factor in the estimate of average annual dose and risk, because the well usage parameter is simply another parameter whose influence can be determined.

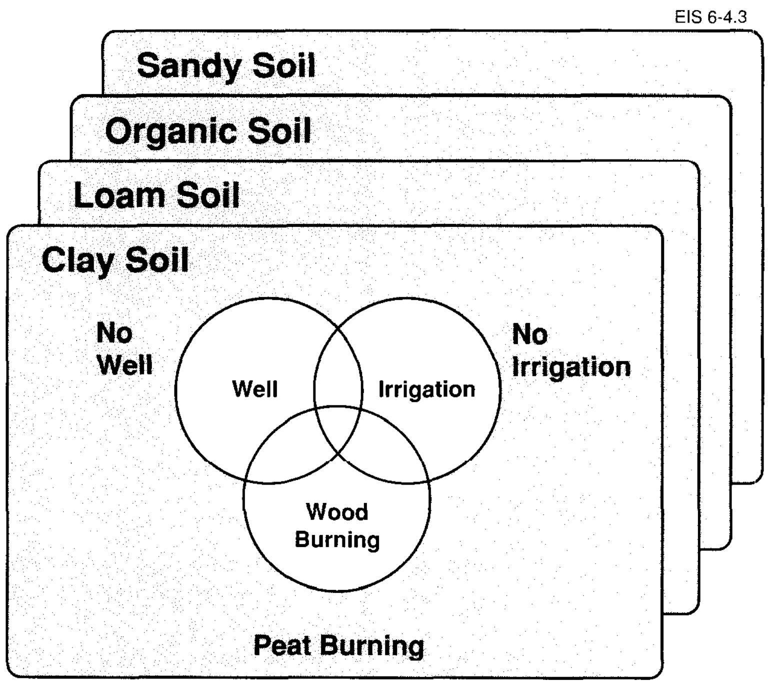

FIGURE 4-3: Combining Scenarios Using Switch Parameters

The circles represent three independent parameters defining mutually exclusive choices:

- a well (or a lake) may be used as the source of domestic water,
- irrigation of the garden may (or may not) be practised, and
- wood (or peat) may be used as a source of heating fuel.

The four layers shown represent another parameter that we assume has four mutually exclusive choices: the soil type may be clay, loam, organic or sandy soil. In all, there are 2 x 2 x 2 x 4 = 32 different possibilities. These 32 possibilities, or scenarios, are analyzed together in SYVAC3-CC3, using four switch parameters.

Although we have included as many factors as possible in the SYVAC scenarios, we have also recognized that it may be desirable to estimate impacts from some particular subset of possibilities. This capability was allowed for during the construction of SYVAC3-CC3. If desired, we can interrogate the complete set of simulation results to extract results from selected simulations. By way of example, we can calculate the average annual dose for the simple situation in which the critical group obtains its drinking water from a well. We can also calculate the average annual dose for the more complex situation in which the soil type is clay, irrigation is practised, a well is used as the source of domestic water, and wood is used as the source of heating fuel.

4.1.5 Screen the Scenarios

The set of scenarios from step 4 was reviewed to identify those that require quantitative evaluation in the postclosure assessment.

This screening step played an important role in the scenario-analysis procedure that led to the results summarized here. Interim screening dealt with a number of possible scenarios (such as a high-demand well scenario), which are now included within the SYVAC scenarios (Goodwin et al. 1994).

We concluded that all three scenarios require quantitative evaluation, and they are therefore examined in Chapter 6. Note that this conclusion applies specifically to the reference disposal system; results may be different for another disposal system.

4.1.6 Detail the Scenarios

This last step in scenario analysis has two objectives: to define more precisely the scenarios requiring quantitative evaluation and to determine how they should be handled in the postclosure assessment.

The following three sections outline the SYVAC, open-borehole, and disruption scenarios. More details are provided in Chapter 5 for the SYVAC scenarios and in Sections 6.7 and 6.8 for the open-borehole and disruption scenarios.

4.2 THE SYVAC SCENARIOS

The SYVAC scenarios contain most of the factors listed in Table 4-2 and are focussed on groundwater-mediated processes affecting the performance of the reference disposal system. We conservatively assume their probability of occurrence is unity in the calculation of risk.

In the SYVAC scenarios, groundwater in the rock surrounding the disposal vault saturates the buffer and contributes to the corrosion of the titanium containers. The groundwater thus controls the release of contaminants and their transport through the engineered and natural barriers to the surface environment. Specific pathways to the surface include fracture zones and a water-supply well that could intercept the contaminated groundwater, including a high-demand well that might substantially alter existing groundwater flow patterns. Once in the surface environment, the contaminants could potentially cause radiological or chemical toxicity effects if they were to come in contact with people or other organisms at sufficiently high concentrations. Other factors in the SYVAC scenarios include contaminant pathways in the biosphere and the properties of the critical group.

Chapter 5 describes how the SYVAC scenarios have been modelled for the reference disposal system. More details of the models and data are given in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993). Results from the quantitative evaluation of the SYVAC scenarios are described in Sections 6.2 to 6.6.

4.3 THE OPEN-BOREHOLE SCENARIOS

The open-borehole scenarios describe a situation in which one or more open boreholes pass near the vault from the surface. They also contain all the factors in the SYVAC scenarios; for example, they include a critical group that obtains its food and water from local sources.

Open boreholes could have significant local perturbations on the groundwater flow fields in and near the disposal vault. They could also provide important pathways affecting the movement of contaminants from the disposal vault to the biosphere.

Plans to decommission and close the disposal facility include the careful sealing of all boreholes, but there is a possibility that one or more deep boreholes may remain open after closure. We could not quantify an associated probability of occurrence at the time the scenario was first identified. However, we show in our analysis of the open-borehole scenarios that they would not contribute significantly to the radiological risk, because three quality assurance procedures would minimize the likelihood that a borehole would remain open at the time of vault closure. (In reaching this conclusion, we make use of quantitative results obtained for the SYVAC scenarios.) Our analysis of the open-borehole scenarios is documented in Section 6.7.

4.4 THE DISRUPTION SCENARIOS

We identified only one disruptive event, inadvertent human intrusion, that is likely to contribute significantly over 10^4 a to the risk associated with the reference disposal system. Its probability of occurrence is extremely small, less than 5×10^{-6} for all times up to 10^4 a (Section 6.8), so that just one such event needs to be evaluated. The corresponding scenarios are called the inadvertent human intrusion scenarios.

The inadvertent human intrusion scenarios describe activities involving drilling, mining or blasting that are carried out in the vicinity of the disposal vault. We assume that the intruder is not aware of the presence of the disposal vault and its potential hazards. We do not include a number of possibilities in these scenarios.

- We exclude deliberate intrusion that might occur if, for example, some group attempted to recover the materials in the vault. We assume that a society desiring these materials would be aware of and capable of dealing with the hazards involved.

- We also exclude the construction and use of a water well. This situation is included in the SYVAC scenarios, where we assume that the critical group may obtain their domestic water and irrigation water from a well, and that the well may intercept a contaminated groundwater plume.

Humans have the potential to inadvertently by-pass all or some of the natural and engineered barriers and may come into direct contact of the waste by moving material from the disposal vault into the surface environment. Merrett and Gillespie (1983) concluded that such activities would be unlikely because the disposal vault is relatively small compared with the total area of the Shield, it is located at a great depth, and it would be sited in rock that is of low economic value. (One of the siting criteria for the vault will be the absence of any mineral or other valuable resources (Eedy and Hart 1988, Davison et al. 1994a).)

Section 6.8 describes our analysis for times up to 10^4 a. It includes an outline of the system model used to estimate impacts and a discussion of these impacts.

5. DESCRIPTION OF MODELS AND DATA

5.1 OVERVIEW OF THE SYSTEM MODEL

5.1.1 Introduction

In Chapter 2, we pointed out that mathematical models are developed and then used to provide quantitative estimates of impacts for the postclosure assessment. The models must represent the entire disposal system, accounting for all factors identified by scenario analysis (Chapter 4) as important to the safety of the concept.

Ideally, the models (and associated data) would provide an accurate and quantitative description of the behaviour of the entire disposal system. This goal is not always possible because we must extrapolate and extend our current understanding far into the future. In developing these models and data, we often introduce simplifications and assumptions, but when we do so they are generally chosen so as to overestimate impacts. We believe the overall effects of the simplifications and assumptions are such that the system model and associated data overestimate the potential impacts.

In the sections that follow, we present an overview of the system model and associated data for the SYVAC scenarios (discussed in Section 4.2) that are assessed in this study of the reference disposal system. The system model is a sequential chain of mathematical models used to describe the behaviour of the vault, geosphere and biosphere components of the disposal system. It is used to estimate impacts and to identify features important to long-term safety. The model and data are implemented under the control of the computer code SYVAC3 (described in Section A.3 of Appendix A).

The system model and data described below (and in Sections 5.2 to 5.8) represent the reference disposal system for the SYVAC scenarios. More detailed discussion on the models and data are provided in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993). These primary references include discussion of the assumptions made in constructing the models and justification of the data used in the models.

5.1.2 Development of the System Model

The system model and data have been developed and refined over many years; earlier versions (not necessarily based on studies at the WRA) have been documented elsewhere (Wuschke et al. 1981, 1985; Heinrich 1984b; Heinrich and Andres 1985; LeNeveu 1986; Mehta 1985; Goodwin et al. 1987a,c; Garisto and LeNeveu 1989, 1991; Engel et al. 1989; Chan et al. 1991). The model and data used in this assessment represent the state of development for the reference disposal system at the end of 1992. Further development would occur as more information becomes available. Changes would certainly be required for the assessment of an actual site being considered for disposal.

The development of the models and data is guided by three Model Working Groups, one for each of the vault, geosphere and biosphere models, which make up the system model. The members of the groups, experts in the relevant scientific and engineering disciplines, established the contents of their respective parts of the system model and the interconnections with other parts. For example, the groups have concurred that the heat generated by the vault will not significantly alter temperatures in the surface environment. Thus they have indicated that the system model need not evaluate the effects of temperature rises in the biosphere near the vault. On the other hand, the vault model Working Group has recommended that elevated temperatures in the vault must be considered for effects on container corrosion. The recommendations and decisions of the Model Working Groups are fully documented in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993).

5.1.3 Features of the System Model

The system model of the reference disposal system is fully integrated and includes all the important factors identified for the SYVAC scenarios as relevant to the quantitative safety assessment for times up to 10^4 a. It provides estimates of environmental impacts, notably annual radiation dose to members of the critical group. This estimated annual dose can then be used to calculate the radiological risk for comparison with the risk criterion (AECB 1987a). The system model also provides estimates of annual radiation dose to other organisms and concentrations of contaminants in the biosphere for evaluation and comparison with other applicable criteria, standards and guidelines, particularly those relevant to assessing environmental impacts.

The system model can also be used to assess the safety-related performance of individual components, such as rate of failure of the containers, and to estimate the location of contaminants in the disposal system at specified times.

One such component of the model of the reference disposal system warrants special mention because it was deliberately introduced to help improve our understanding of its importance to safety. This component, a planar fracture zone in the rock, has been observed at the WRA, the site used as the basis for the geosphere model (Davison et al. 1994b). We have assumed that this fracture zone (referred to as fracture zone LD1) extends to a greater depth than is actually observed, and passes downwards through the plane of the hypothetical vault. Fracture zones are common in plutons on the Canadian Shield; thus our model of the reference disposal system includes LD1. We show in Chapter 6 that its properties are important to the performance of the disposal system and that our assumptions regarding its properties are conservative. From an analysis of its effects, we are able to point to design constraints on the reference disposal system that would lead to improved performance. We use one such design constraint, related to the layout of the vault relative to LD1, to develop a final design of the reference disposal system (Section 6.2).

Figure 5-1 illustrates the system model for the reference disposal system. To simplify the mathematical simulation procedure, we use separate models to describe the vault, geosphere and biosphere, with linkages to connect the vault and geosphere models, and the geosphere and biosphere models. The three models and two linkages, considered together, represent the entire waste disposal system considered in the postclosure assessment of the SYVAC scenarios.

The three models simulate the processes described below.

Vault Model: Figure 5-2 and Table 5-1 summarize the properties of the engineered features in the vault that are important in the description of the vault for the reference disposal system. These features include the UO_2 fuel pellets, used-fuel bundles, containers, buffer and backfill.

The vault model simulates these features with mathematical equations (Johnson et al. 1994b) that describe

- the inventories of contaminants in the UO_2 fuel matrix and Zircaloy fuel sheaths, which change as a function of time due to radioactive decay;

- the corrosion of the containers that eventually leads to penetration by groundwater and the release of contaminants;

- the release of contaminants dissolved in groundwater to the buffer from the UO_2 fuel matrix and the Zircaloy fuel sheaths. This release starts when a container fails (we assume that the Zircaloy sheaths would fail relatively quickly, and thus they would not offer additional protection to the fuel matrix);

- the transport of contaminants in groundwater through the buffer and backfill; and

- the net release of contaminants in groundwater to the rock surrounding the vault.

The link between the vault and geosphere models ensures that groundwater movement near and inside the vault, and contaminant movement out of the vault, are consistent with the hydrogeological conditions in the surrounding geosphere.

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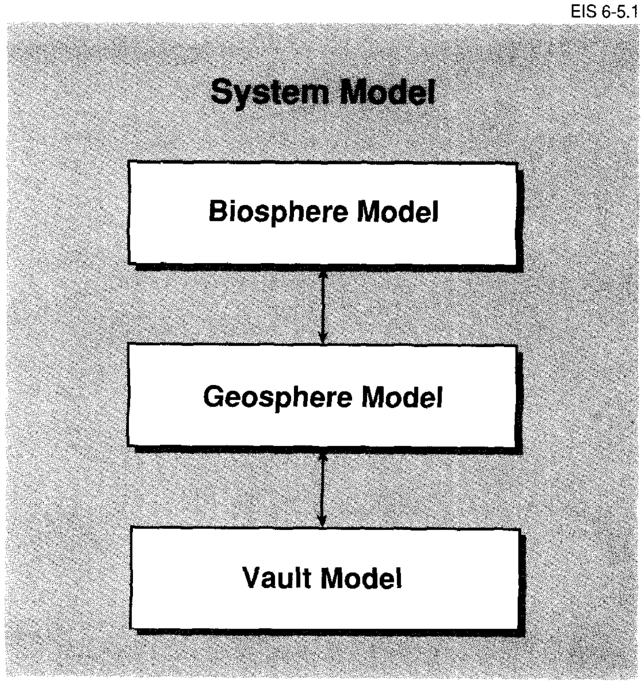


FIGURE 5-1: Illustration of the System Model for the Reference Disposal System

The system model contains all features judged to be important for the SYVAC scenarios that are examined for the reference disposal system and used to estimate the performance and safety of the entire system. It consists of three linked models representing the vault, geosphere and biosphere. The vault model simulates the release of contaminants from the containers and waste form and their transport through buffer and backfill to the rock surrounding the vault. The geosphere model simulates the transport of contaminants from the vault through the rock of the geosphere to discharge zones in the biosphere. The biosphere model simulates the transport of contaminants in the water, air and soil of the biosphere and estimates subsequent impacts, such as annual radiation dose to individuals of the critical group and to nonhuman biota. Information from an extensive research and development program is used to formulate the models and to provide data for the models.

The linkage between models is represented by two-headed arrows connecting the models and showing that information can flow both ways. For example, groundwater flow characteristics in the geosphere model affect the release of contaminants from the vault model, and contaminant releases from the vault are used in the geosphere model. Similarly, usage of a well by the critical group in the biosphere model affects groundwater flow to the well in the geosphere model (and can even affect groundwater flow near the vault), and the characteristics of the geosphere model affect the ability of the well to supply water.

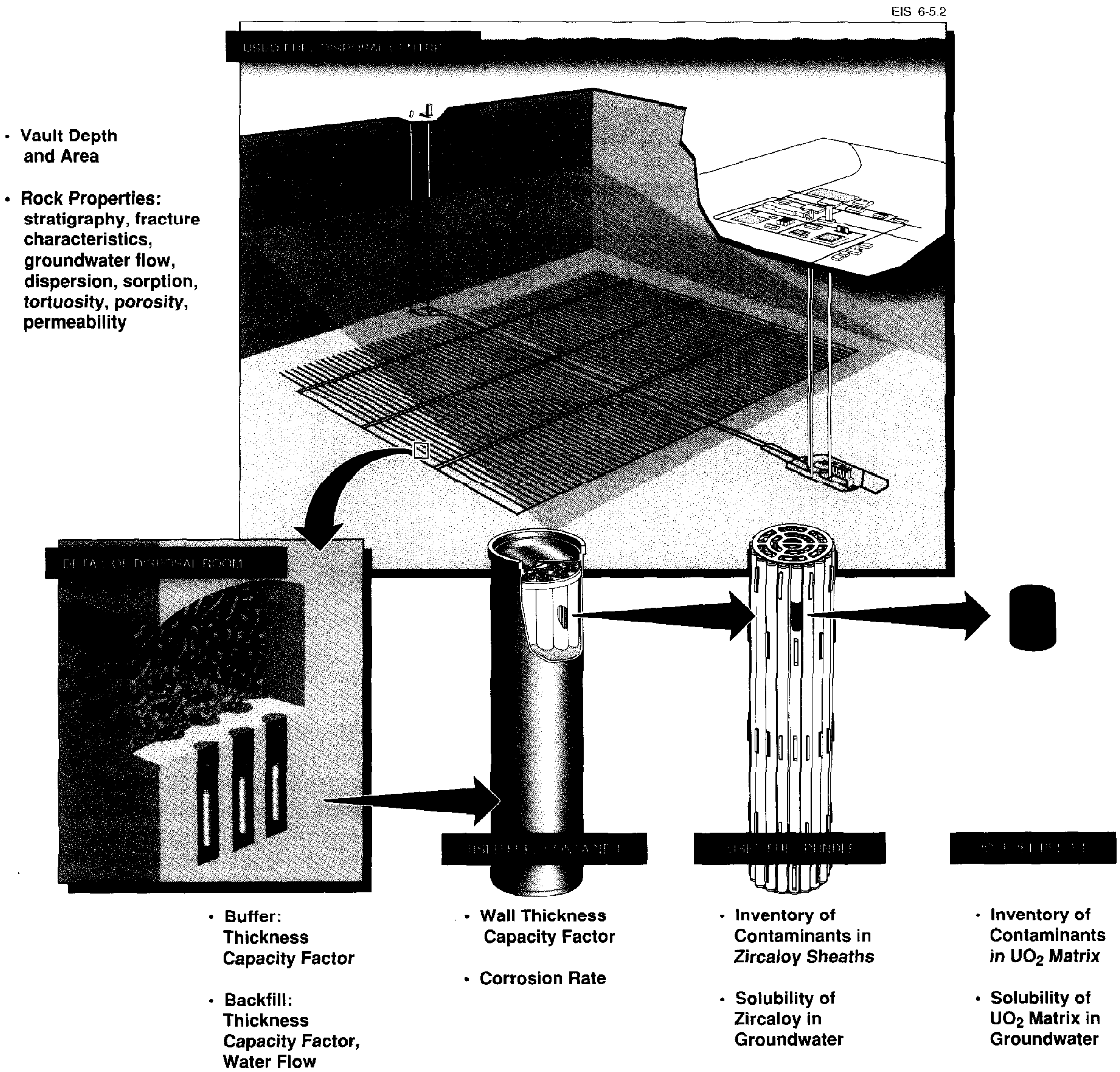


FIGURE 5-2: Important Engineered Features and Natural Barriers

This figure illustrates the different scales of barriers in the disposal system and lists some of their important properties. The UO_2 fuel pellet, for example, is an effective barrier because it would dissolve very slowly in groundwater, and thereby inhibit the release of contaminants. Its important properties include the solubility of the UO_2 matrix and the inventory of contaminants associated with used fuel. A summary of the properties and associated models for these barriers is provided in Sections 5.2 through 5.6, with more detail in the primary references for the vault model (Johnson et al. 1994b) and the geosphere model (Davison et al. 1994b).

TABLE 5-1

PROPERTIES OF ENGINEERED FEATURES AND NATURAL BARRIERS USED IN THE VAULT AND GEOSPHERE MODEL CALCULATIONS*

Properties of Engineered Features and Natural Barriers	Model Calculations
UO_2 Fuel Pellets Initial contaminant inventory in the UO_2 matrix, half-life	Inventory of contaminant in UO_2 matrix as a function of time
Solubility of UO_2 matrix in groundwater	Contaminant-release rate from the UO_2 matrix once a container has failed
Used-Fuel Bundles Initial contaminant inventory in Zircaloy, half-life	Inventory of contaminant in Zircaloy as a function of time
Solubility of Zircaloy matrix in groundwater	Contaminant-release rate from Zircaloy once a container has failed
Used-Fuel Container Thickness of container wall, corrosion rate, initial defects	Container failure as a function of time Congruent-release rate of contaminant to the buffer
Inventory of instant-release contaminant; half-life; volume and surface area of container	Instant-release rate of contaminant to the buffer
Buffer Layer Buffer thickness, contaminant solubility, capacity factor, half-life	Contaminant-release rate to the backfill and to the surrounding rock
Backfill Layer Backfill thickness, permeability tortuosity; water velocity; contaminant capacity factor, half-life	Contaminant-release rate to the surrounding rock
Vault Location Distance to nearby geological features, vault sectors, vault depth, characteristics of the surrounding rock	Net contaminant release from all parts of the vault to the geosphere
Rock Layers, Fracture Zones, Well Rock thickness, porosity, tortuosity, permeability, dispersivity; well depth and demand; contaminant retardation factor, diffusion coefficient, half-life	Groundwater velocities near the vault, volumetric flow rate to the biosphere, and contaminant-release rates to the well and surface discharge zones

* The left-hand column lists important properties of the engineered features and natural barriers of the reference disposal system (see also Figure 5-2). The right-hand column shows how they are used in the model calculations. The properties of the UO_2 pellets, for example, include the initial inventories of contaminants. These properties, along with radioactive half-lives of radioactive isotopes, are used to calculate the amount of contaminants in the fuel pellet as a function of time.

Geosphere Model: Figure 5-2 and Table 5-1 summarize the properties of the barriers that are important in the geosphere model of the reference disposal system. One important barrier is the extensive mass of rock that isolates the vault from the biosphere, which is a function of the vault depth. Another important feature is the location of the vault relative to nearby geological features. As noted earlier, for the reference disposal system, we have assumed that the hypothetical vault is located near a fracture zone, LD1. Moreover, we have assumed that LD1 extends downwards past the plane of the vault and has good hydraulic connections with other features (Davison et al. 1994b). Our analysis (Chapter 6) shows that the distance separating the vault and LD1 has a strong influence on the safety of the disposal system.

The geosphere model uses mathematical equations (Davison et al. 1994b) to describe

- groundwater movement through the rock surrounding the vault and the overburden near the surface of the rock mass, including preferential movement through fracture zones and the effects of drawing water from a well;

- the movement of contaminants in the groundwater in the geosphere; and

- the net release of contaminants into the biosphere at a well and surface discharge zones (three surface discharge locations are modelled for the reference disposal system).

The link between the geosphere and biosphere models ensures that both models are consistent with respect to groundwater and contaminant movement. It also ensures that well-water demand does not exceed the capacity of the groundwater flow system to supply water.

Biosphere Model: The features of the biosphere model are summarized in Figure 5-3 and Table 5-2. Figure 5-4 shows the major pathways of contaminant transfer through the geosphere and the biosphere to man, based on our analysis for the reference disposal system (described in Chapter 6).

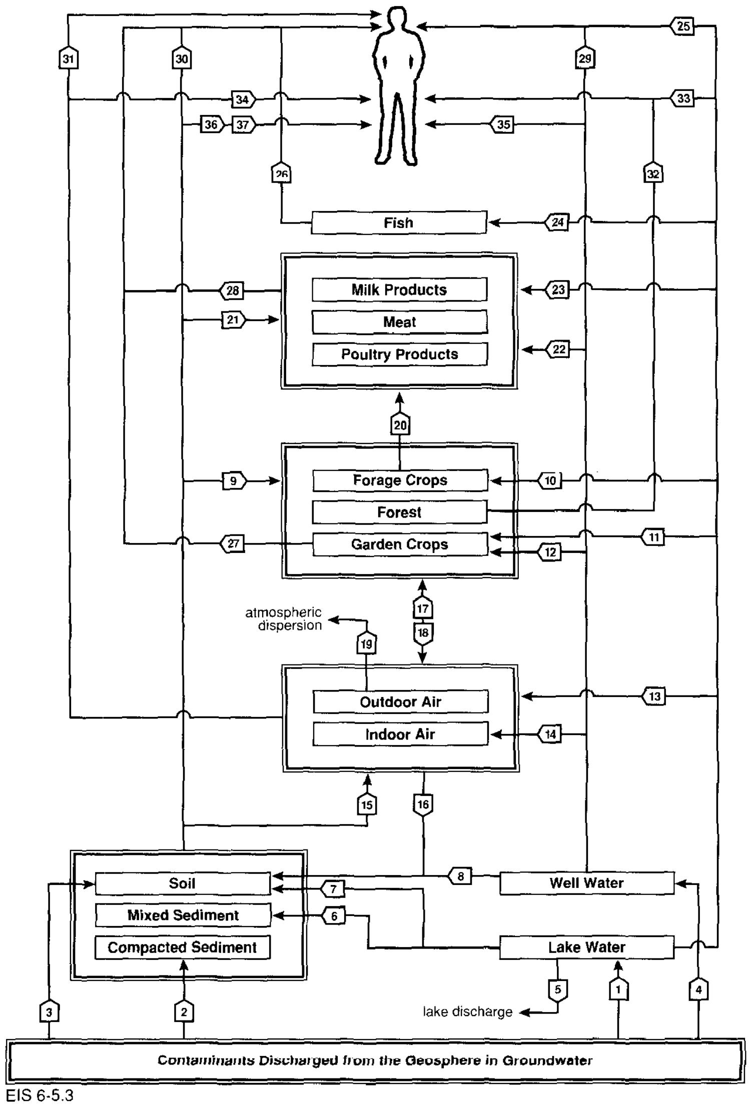
The biosphere model uses mathematical equations (Davis et al. 1993) to

- describe the movement of contaminants through soil, plants and animals, the water and sediment of a lake, and the local atmosphere near the discharges from the geosphere;

- estimate the concentrations of contaminants in the soil, water and air in the local habitat of the critical group and other biota;

- estimate annual radiation dose to an individual in the critical group caused by ingestion and inhalation of the contaminants and by exposure to radiation from contaminants in the environment; and

- estimate radiation doses to nonhuman biota.



The numbered arrows indicate the direction of movement:

- 1 to 4 are discharges from the geosphere to lake water, compacted sediment, soil and well water.
- 5 and 19 identify losses from the biosphere through lake discharge and atmospheric dispersion.
- 6, 7, 10, 11, 13, and 23 to 25 are transfers from the lake to mixed sediments, to soil (irrigation), to leaves of forage and garden crops (irrigation), to air, to terrestrial animal products, to fish and to man (ingestion).
- 8, 12, 14, 22, and 29 are transfers from well water to soil (by irrigation), to leaves of garden crops (irrigation), to indoor air, to terrestrial animal products and to man (ingestion).
- 9, 15, 21, and 30 are transfers from soil and sediment to plants (root uptake), to air, to terrestrial animal products and to man (ingestion).
- 16, 17, and 31 are transfers from air to soil (deposition), to plant leaves (deposition) and to man (inhalation).
- 18, 20, and 27 are transfers from plants to air, from forage crops to terrestrial animal products, and from garden crops to man (ingestion).
- 26 is the transfer from fish to man (ingestion).
- 28 is the transfer from terrestrial animal products to man (ingestion).
- 32 to 37 show external exposure routes to man, involving exposure to wooden building materials, lake water, air, well water, soil and sediments, and inorganic building materials.

FIGURE 5-3: The Main Transfers Through Which Contaminants Move from the Geosphere into the Biosphere and to Man (the numbered arrows indicate the direction of movement)

TABLE 5-2

PATHWAYS IN THE BIOSPHERE CONSIDERED IN THE SYSTEM MODEL*

Pathway	Description
Uptake from Soil 1. Soil/plant/meat/man 2. Soil/plant/milk/man 3. Soil/plant/bird/man 4. Soil/plant/man	- Used to estimate dose to man from the ingestion of animal products and plants, arising from the uptake of contaminants from soil
Atmospheric Deposition 5. Air/plant/meat/man 6. Air/plant/milk/man 7. Air/plant/bird/man 8. Air/plant/man	- Used to estimate dose to man from the ingestion of animal products and plants, arising from the deposition of contaminants on plant leaves (includes deposition from irrigation water)
Ingesting Water 9. Water/meat/man 10. Water/milk/man 11. Water/bird/man 12. Water/man	- Used to estimate dose to man from the ingestion of animal products and water, arising from contaminated drinking water and irrigation water
Ingesting Soil 13. Soil/meat/man 14. Soil/milk/man 15. Soil/bird/man 16. Soil/man	- Used to estimate dose to man from the ingestion of animal products and soil, arising from direct intake of contaminated soil by the animal or man
Other Internal Routes 17. Fish/man 18. Inhalation	- Used to estimate dose to man from the ingestion of fish from a contaminated lake and from the inhalation of contaminated air
External Routes 19. Air 20 Water 21. Ground 22. Wood 23. Inorganic	- Used to estimate external doses to man from immersion in contaminated air and water, reflection from contaminated ground (groundshine), and exposure to buildings constructed of wood and inorganic material

* This table identifies the 23 pathways that are simulated in the biosphere model for the reference disposal system and that would lead to impacts to an individual of the critical group. For example, the first pathway involves contaminant transport from soil to plants, from plants to the edible meat of animals, and from meat to man (the arrows numbered 9, 20 and 28 in Figure 5-3). To describe this pathway, the biosphere model uses parameters such as soil type and depth and transfer factors from plants to animal meat to estimate contaminant concentrations in animal meat, and parameters relating to diet to estimate radiation dose to an individual in the critical group. The source of contamination is groundwater from the geosphere, which may enter the biosphere at the lake, the soil and sediment, or the well (Figure 5-3).

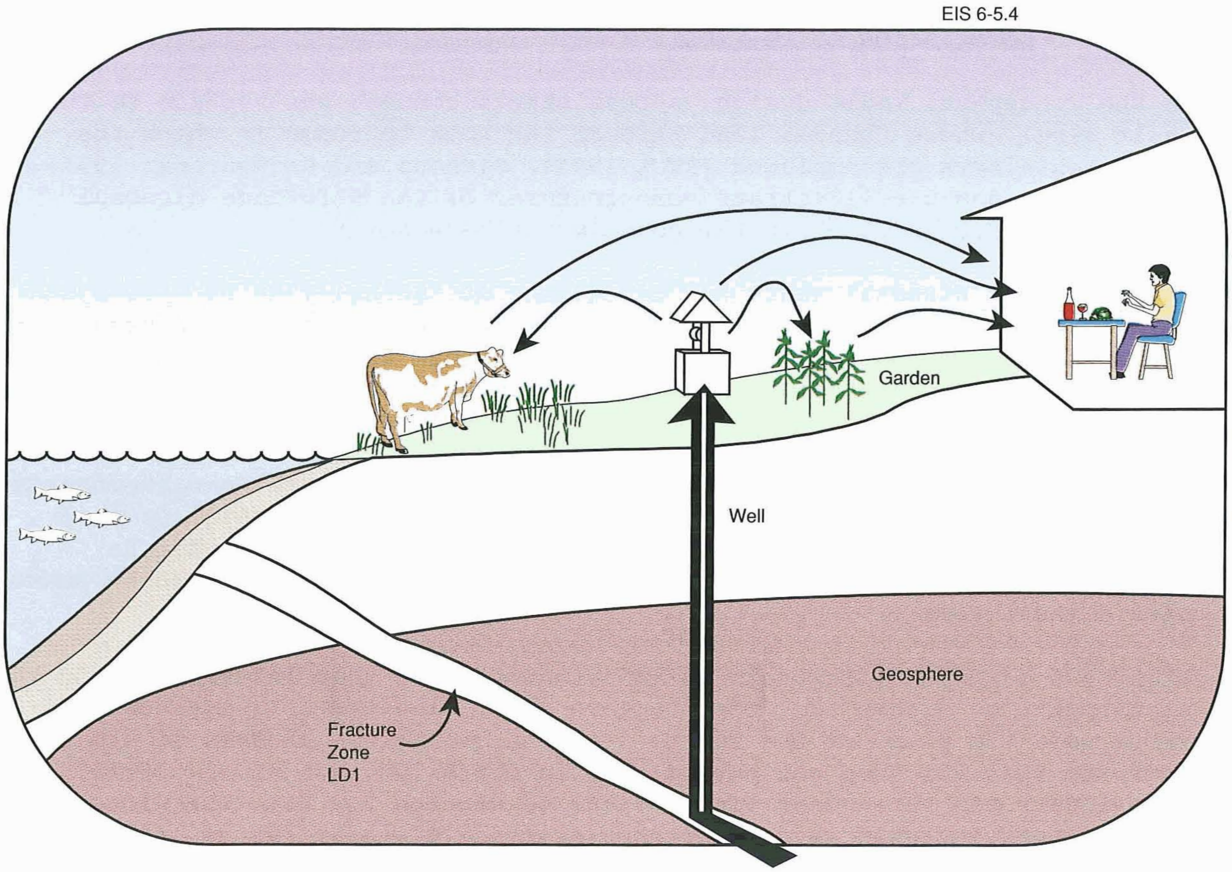


FIGURE 5-4: Major Pathways in the Biosphere

The arrows indicate the pathways found to be important in this assessment. One such pathway leads from the vault through a region of sparsely fractured rock to fracture zone LD1, to the well, to plants through irrigation of a garden with well water, and then to humans who consume the plants as food. Another involves ingestion of well water. Other pathways, such as inhalation of contaminated air, are included in the system model but do not appear in this figure because they are less important.

We use these estimates of contaminant concentrations and annual doses to evaluate the expected impacts of the reference disposal system on public health and the environment.

5.2 DESCRIPTION OF THE VAULT MODEL

This section describes the main features of the vault and vault model that are important for the postclosure assessment of the SYVAC scenarios for the reference disposal system. Further details, including justification of the assumptions and data used by the model, are provided in the primary reference for the vault model (Johnson et al. 1994b).

5.2.1 Description of the Vault

In the conceptual vault design, access shafts connect the surface to the vault level, where tunnels lead through the rock to rooms in which the waste containers are emplaced (AECL 1994a, Simmons and Baumgartner 1994). Figures 5-5 and 5-6 illustrate some features of the reference disposal system that are analyzed in the postclosure assessment.

The reference disposal vault has dimensions of (about) 1700 by 1900 m and is at a depth of about 500 m. These dimensions are slightly different from those in the general concept (AECL 1994a, Simmons and Baumgartner 1994), for reasons discussed below. During operation of a disposal vault, there would be both surface and subsurface facilities. We assume in the post-closure assessment that the surface facilities have been removed. We also assume that shafts and boreholes leading to the vault have been thoroughly sealed and that all vault rooms, tunnels and subsurface facilities have been backfilled. (The open-borehole scenarios, discussed further in Section 6.7, examine a situation in which we assume an open borehole passes near a vault room.)

Figures 5-5 to 5-7 illustrate an important feature that is evaluated in the assessment: we assume that the fracture zone, labelled LD1, extends down-wards past the plane of the vault. (Recent geological studies of the WRA indicate that LD1 does not extend to this depth (Davison et al. 1994b), and we evaluate the subsequent implications in Section 8.2.6.) The presence of LD1 has been included as part of the reference disposal system, so that we could examine how a nearby extensive fracture zone could affect the perfor-mance of the disposal system.

Figures 5-5 and 5-6 show that the lengths of the rooms nearest LD1 are shorter than the other rooms. These shortened lengths and the position of the vault relative to LD1 are made so that there exists a region of rock between the rooms toward the right-hand end of the vault and the fracture zone. The closest distance in a horizontal direction from LD1 to the waste emplacement part of any room is about 150 m, but the closest perpendicular distance is only about 50 m (see Figure 5-7) because the plane of the fracture zone is inclined at a shallow angle of about 18° relative to the plane of the vault, passing above the vault (Davison et al. 1994b). We refer to this 50 m as the waste exclusion distance. Geological observa-tions indicate that the rock within this zone is relatively free of frac-tures and has a low permeability. (Detailed engineering drawings of the vault layout relative to fracture zone LD1 show that the closest horizontal and perpendicular distances are 150.5 and 46.5 m respectively. We use these more precise values in our calculations.)

We considered several options to achieve this waste exclusion distance. We started with the description of the vault in the general concept, for which the vault is 2000 m^2 and contains 191 000 Mg U (AECL 1994a, Simmons and Baumgartner 1994). For this postclosure assessment study, we chose to eliminate that portion of the disposal vault near LD1, such that there would be a waste exclusion distance of about 50 m and such that the vault rooms are beneath LD1. This choice allowed for the best use of available geological and hydrogeological information in the vault model. However, it

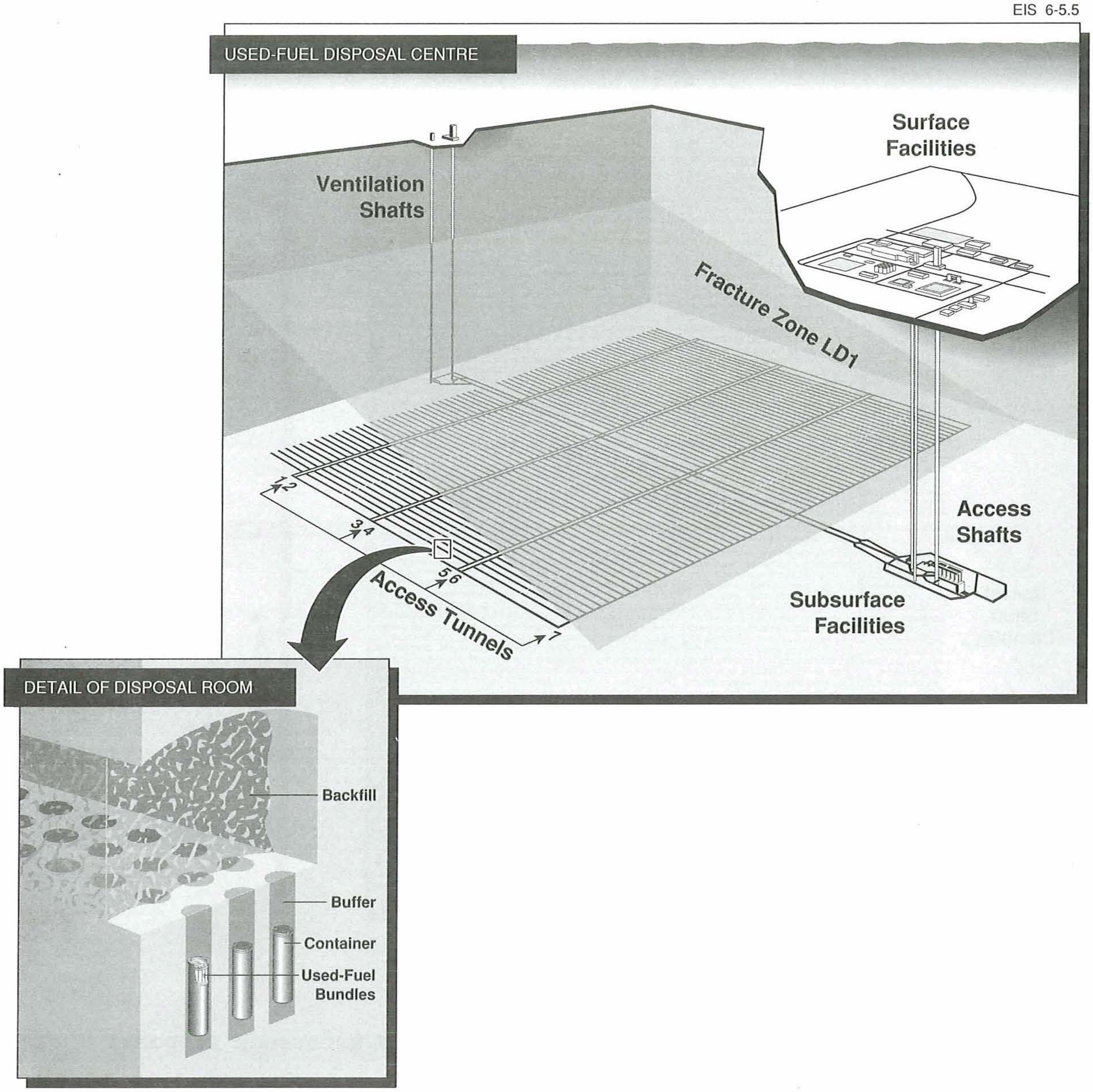


FIGURE 5-5: The Design of the Vault for the Reference Disposal System

The vault is about 500 m below the surface and consists of numerous tunnels and shafts and a total of 434 disposal rooms that are entered through 7 access tunnels (some detail cannot be resolved using the scale in the figure; for example, the rooms leading from access tunnel 2 do not connect with those from access tunnel 3). The inset illustrates a cross section of a typical disposal room.

The rooms leading from access tunnel 7 are shorter than the other rooms (see also Figures 5-6 and 5-7). The location of the vault is such that there is a region of rock about 150 m long (horizontally) between fracture zone LD1 and the waste emplacement part of the nearest room. However, the plane of LD1 is inclined at a shallow angle, so that the closest perpendicular distance to LD1 is only about 50 m. This is the waste exclusion distance, designed to isolate nuclear fuel waste from LD1.

For the postclosure assessment, we assume that all surface facilities have been removed, the shafts have been completely sealed, and all rooms, interconnecting tunnels and subsurface facilities, have been backfilled.

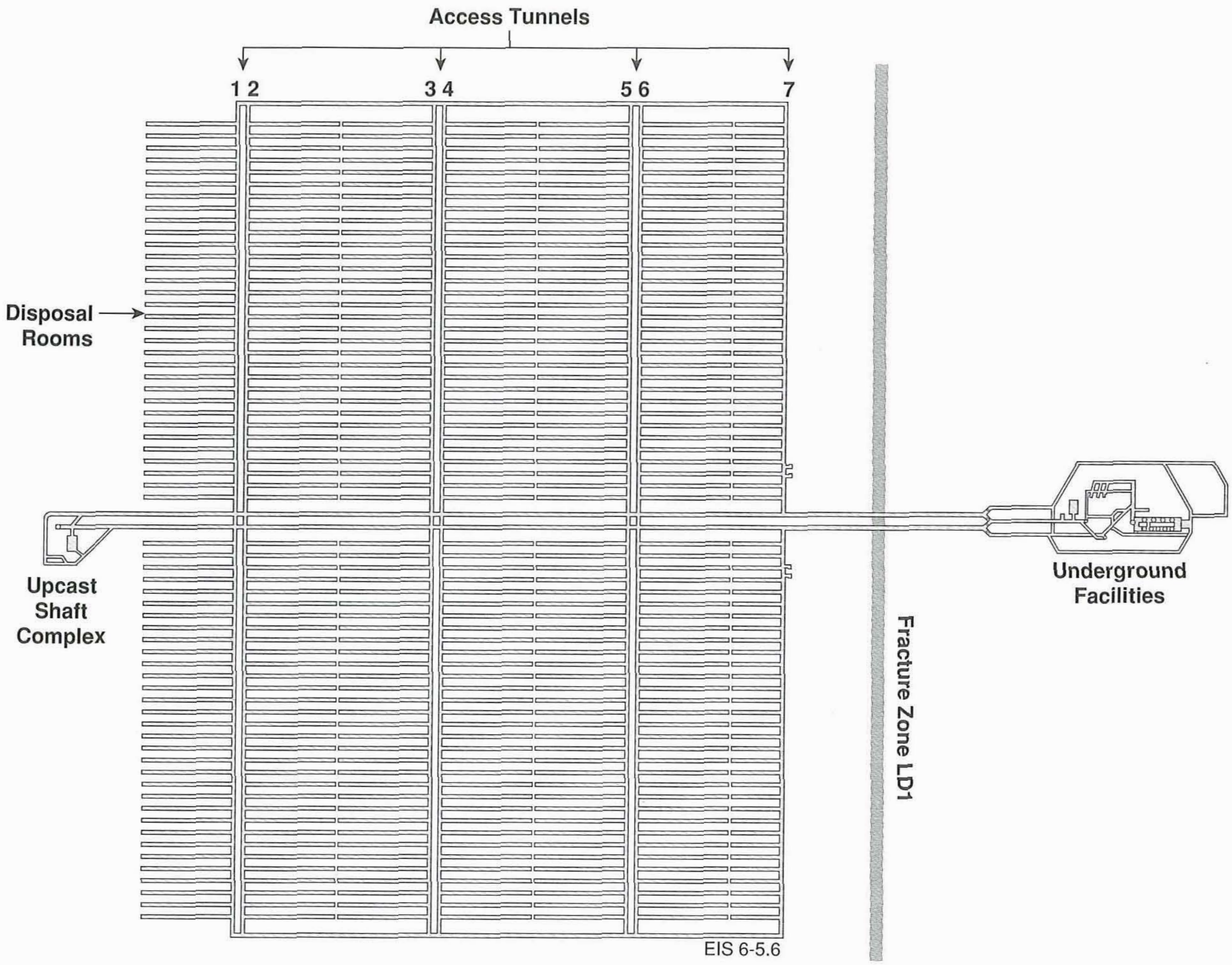


FIGURE 5-6: Overhead View of the Vault for the Reference Disposal System

The vault consists of 434 disposal rooms (note the short length of rock separating rooms such as those entered from access tunnel 2 and those entered from access tunnel 3). Most rooms are 234 m long, with 200 m for waste emplacement and 34 m for bulkheads. The exceptions are the rooms leading from access tunnel 7, which have a waste emplacement area only 105 m long. We assume in the postclosure assessment that all excavated openings are backfilled and sealed, including the access tunnels, disposal rooms, upcast shaft complex and underground facilities.

A waste exclusion distance of about 50 m isolates fracture zone LD1 from the waste emplacement part of the rooms closest to LD1. To achieve this waste exclusion distance, we have chosen an option (discussed in Section 6.2) in which vault rooms nearest the fracture zone are shortened (to 105 m), with an associated change to the vault dimensions.

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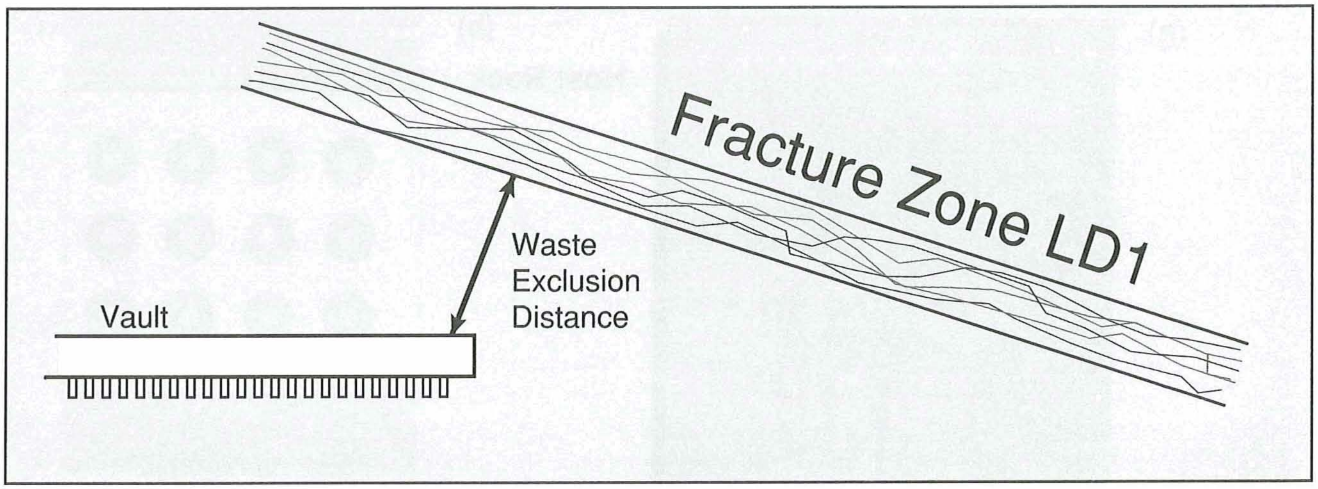

FIGURE 5-7: Cross Section of a Vault Room Located near Fracture Zone LD1

This cross section illustrates some detail of a vault room closest to fracture zone LD1 for the reference disposal system. The waste exclusion distance is the length of the interposing region, containing sparsely fractured rock, that isolates the waste emplacement part of a room from the fracture zone. The distance in a horizontal direction from a container in the rooms closest to LD1 is about 150 m; however, the nearest distance is about 50 m because LD1 is inclined at a shallow angle (about 18°) to the plane of the vault.

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also corresponds to a vault that is smaller in size than that described by Simmons and Baumgartner (1994) and to a reduced inventory of uranium, 162 000 Mg U. Section 6.2 discusses the analyses related to this choice.

Figure 5-8 shows details of a vault room of the reference disposal system that contains the nuclear fuel waste. A typical reference disposal system vault room is 200 m long (234 m including bulkheads), 8 m wide and 5.5 m high at the centre. Rooms nearest LD1 are smaller (105 m long). Each room contains boreholes in the floor, three abreast and separated by 2.1 m (centre to centre). Each borehole, measuring 1.24 m in diameter and 5.0 m long, holds a sealed container made of Grade-2 titanium that accommodates the nuclear fuel waste. A typical vault room has 288 boreholes. Glass beads are used to fill the void space in each container and to provide internal mechanical support. The containers are completely surrounded by a thin layer of sand, which in turn is surrounded by a thicker layer of a low-permeability clay-sand mixture called the buffer.

The clay in the buffer becomes plastic and swells when it is wetted. It would form an impermeable layer, and there would be essentially no flow of

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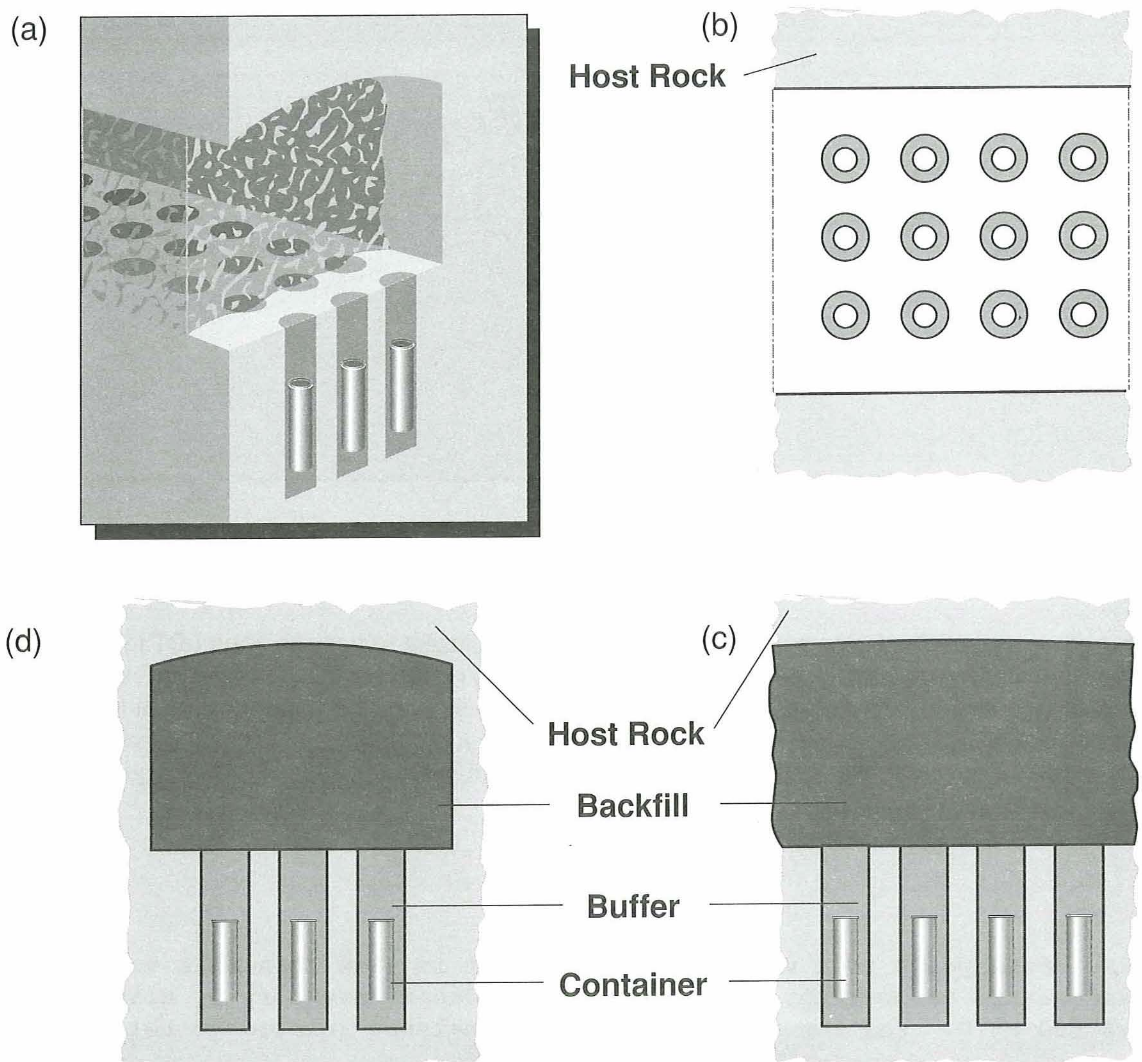

FIGURE 5-8: Four Views of a Typical Disposal Room for the Reference Disposal System

View (a) is a three-dimensional view of part of a room. View (b) is an overhead view, showing the pattern of boreholes drilled in the floor of the room. Views (c) and (d) are cross sections taken down the length and across the width of a room respectively. The waste containers are placed into the boreholes, surrounded by a thin layer of sand (not shown in the figure), which in turn is surrounded by a thicker layer of a low-permeability bentonite clay called the buffer. After closure, the remainder of each room is filled with a mixture of glacial lake clay and crushed rock called the backfill.

water in the buffer. Consequently, the transport of contaminants is effectively limited to very slow diffusion through the water contained within the buffer. Many contaminants also sorb onto the clay, thus further slowing their movement within the buffer.

The spaces in the rooms and tunnels are filled with backfill consisting of a low-permeability mixture of glacial lake clay and crushed rock, and with concrete bulkheads in different locations. All shafts and boreholes are sealed with low-permeability concrete plugs, with the rest of the volume filled with crushed rock, clay and grout. Contaminants could move through the backfill by two mechanisms: by transport in slowly moving groundwater and by diffusion in groundwater away from regions of higher concentration.

We expect that these barrier properties will not change significantly in the vault environment for at least 10^4 a (Johnson et al. 1994b, Davison et al. 1994b), the time frame of concern for quantitative estimates of impact.

5.2.2 Features of the Vault Model

The mathematical description of the vault, or the vault model, is used to simulate the release and transport of contaminants within the vault. It includes the processes in which groundwater that has entered the vault successively corrodes the containers, dissolves the waste, and mediates the movement of contaminants through the buffer and backfill to the rock surrounding the vault.

The model for the reference disposal vault employs characteristics of the vault required to simulate these processes. Some characteristics are related to a simplified geometry of the vault. We identify two important levels of simplification:

- The three-dimensional geometry of the containers, buffer, backfill and surrounding rock is represented as planar layers, and we use only one spatial variable to describe the thickness of each layer (Garisto and LeNeveu 1989). This simplified one-dimensional transport geometry is illustrated in Figure 5-9; contaminant movement is simulated in the direction perpendicular to the planes.

- The reference disposal vault occupies an area of about 3 km^2. On this scale, the surrounding rock is expected to exhibit significant variations in its hydrogeological properties, including variations in the surface topology and variations in subsurface groundwater velocities. These variations could affect contaminant movement in and around the vault. To account for these variations, we divide the vault into distinct sectors, such that the properties of the rock (notably groundwater velocities) adjoining each sector are relatively uniform. Twelve sectors are used for most of the modelling of the reference disposal system.

  Each sector is treated as a plane source (Figure 5-9) and is connected to the geosphere transport pathways (discussed in Section 5.4).

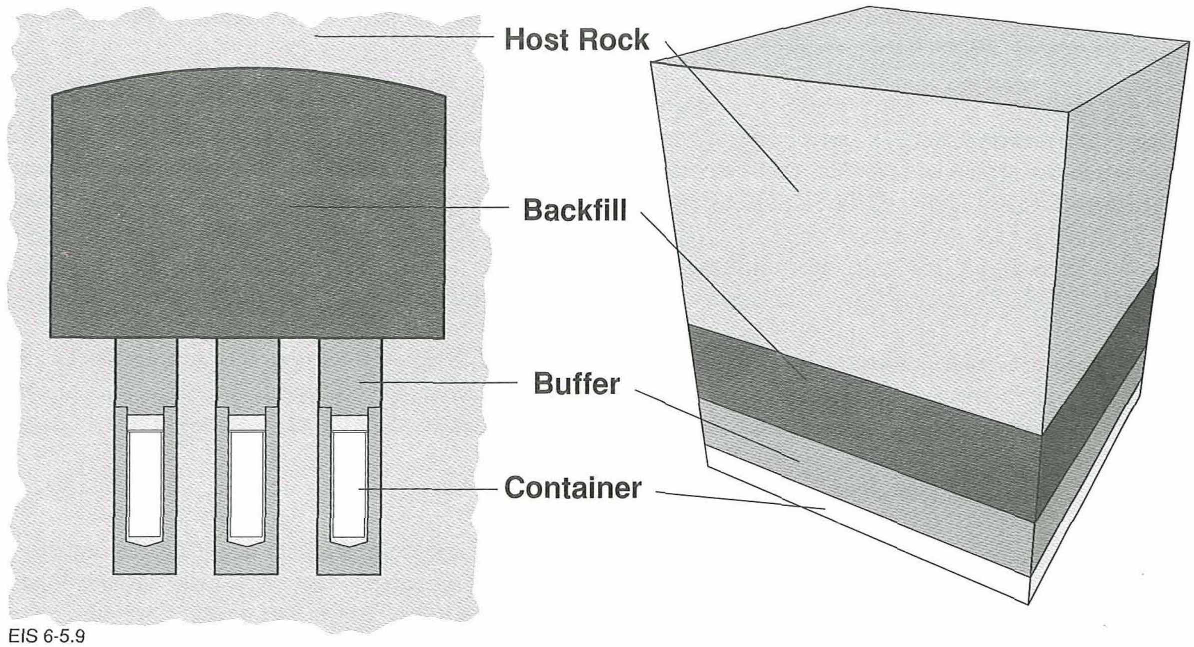

FIGURE 5-9: The Simplified Geometry Used to Represent the Reference Disposal Vault

Contaminants leaving the waste container must pass through the buffer and, possibly, the backfill before reaching the host rock. Each vault sector is approximated as a series of planar layers and contaminant transport is described using only one spatial variable in the direction perpendicular to the planes (Johnson et al. 1994b). The parameters required by the vault model correspond to the effective thickness of the layers representing the buffer, backfill and surrounding rock. Different sectors may have different values (notably for parameters like the mass transfer coefficients).

Two distinct cases are simulated:

- If the backfill is between the buffer and fracture zone LD1, we assume that contaminants travel through both the buffer and the backfill before entering the rock. This is the case for all 12 sectors shown in Figure 5-10. For the simplified vault geometry, the effective thickness of the backfill is taken to be 1.4 m (its actual thickness is up to 5.5 m), to account for the fact that a portion of the contaminants could pass through the rock before encountering the backfill.

- In some special studies (Section 6.2), we assume that there are rooms on both sides of fracture zone LD1. For those rooms located above LD1, the backfill is *not* between the buffer and the fracture zone, and we assume that contaminants from these rooms travel through the buffer and enter the surrounding rock without ever penetrating the backfill.

Figure 5-10 shows the 12 sectors: most are clustered near LD1 because distance to the fracture zone is an important property affecting contaminant transport from a sector. We place more sectors in the region of the vault where these distances are small. (The rationale for the number and location of the sectors is described in the primary reference for the geosphere model (Davison et al. 1994b).) Each sector is allocated a fraction of the waste in proportion to its plan area. The sectors may also have different properties, such as container failure rates and mass transfer coefficients (described below), depending on the location of the sector within the vault. These properties are characterized using different parameter values.

We use the vault model to estimate the release of contaminants from each sector to an adjoining location in the geosphere (Johnson et al. 1994b). The model accounts for the factors important to the transport of contaminants out of a sector, including radioactive decay and ingrowth of radionuclides.

In the following paragraphs, we describe how the processes of waste-form release, container failure and transport of contaminants through the buffer and backfill are simulated by the vault model. We also identify the important parameters used by the model. These processes and parameters are more fully documented in the primary reference for the vault model (Johnson et al. 1994b).

5.2.2.1 Release of Contaminants from the Waste Form

The contaminants of concern are associated with two monolithic structures, or waste matrices: the used-fuel pellets and the Zircaloy fuel sheaths. We model the release of these contaminants assuming they are released by congruent and instant-release processes (Johnson et al. 1994b):

- The majority of the contaminants are embedded in matrices of uranium dioxide and Zircaloy (Garisto et al. 1986). We assume that these matrix-bound contaminants are released upon dissolution of the matrix. The release occurs at a rate determined by the dissolution rate of the matrix and the abundance of the contaminant in the matrix. This is the congruent-release mechanism.

  Important parameters describing congruent release are the inventories of the contaminants in used-fuel pellets and Zircaloy fuel sheaths and the solubilities of the used-fuel pellets and Zircaloy fuel sheaths.

- A fraction of the inventory of some contaminants is located in the gaps and grain boundaries of the fuel pellets and is not bound up in the used-fuel matrix. We assume that this inventory is released to the void spaces within the interior of the container and the sand surrounding the container, immediately upon failure of the container. Thereafter, this inventory slowly diffuses into the buffer. This is the instant-release mechanism

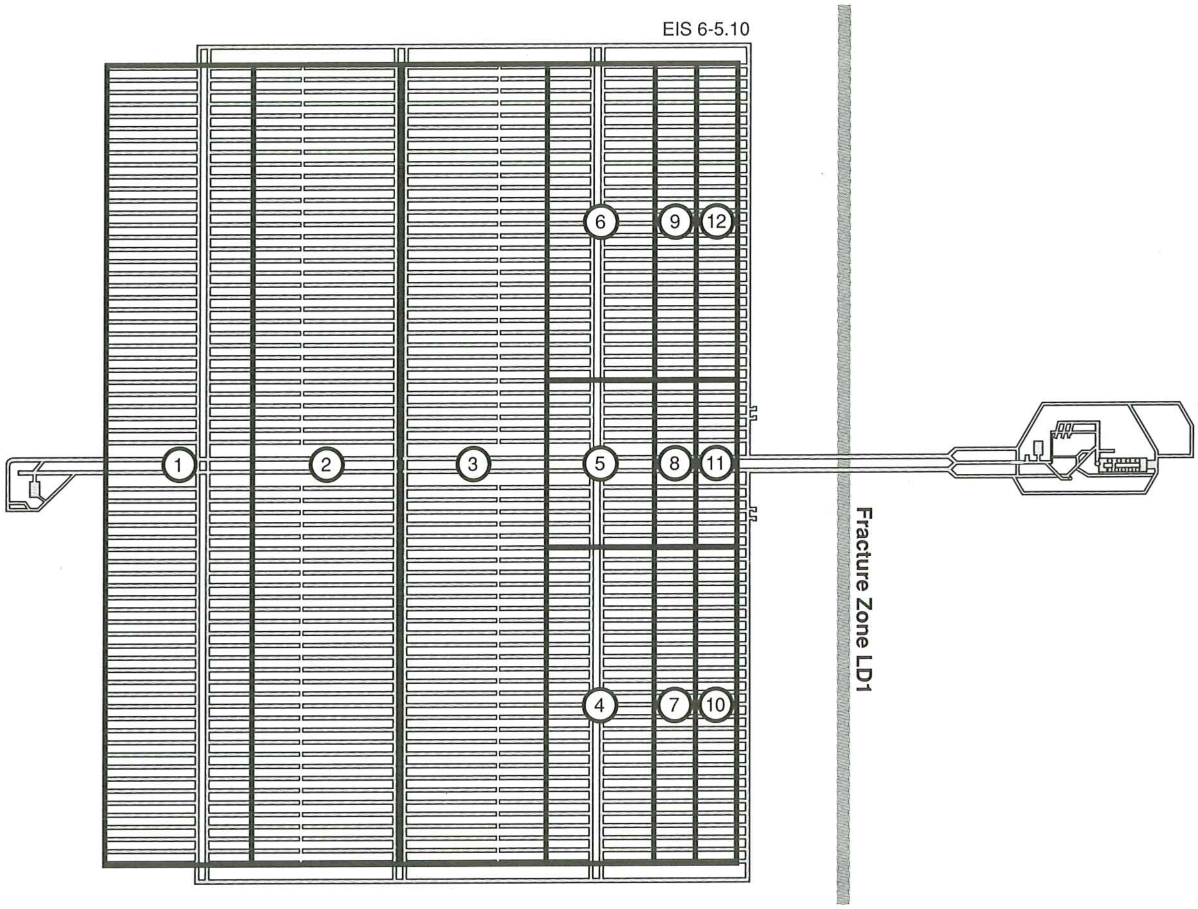

FIGURE 5-10: Overhead View of the Vault for the Reference Disposal System, Illustrating the 12 Sectors

The vault occupies an area of about 3 km^2 and has been divided into 12 sectors. We have made this division on the basis of a groundwater flow field derived from the MOTIF code (Davison et al. 1994b). We assume that the rock adjoining each sector has relatively uniform hydrogeological properties. Most of the sectors are clustered near fracture zone LD1, because the distance to the fracture zone is an important parameter affecting the movement of contaminants from a sector into the surrounding rock.

(Johnson et al. 1994b). As explained above, the remaining fraction of the inventory of these contaminants is released congruently with the dissolution of the used-fuel matrix. (There is no instant release for contaminants in the Zircaloy waste matrix.)

An important parameter describing instant release is the fraction of the inventory, for each contaminant, that is not immobilized within the used-fuel matrix. Radionuclides with significant instant-release fractions are ^{39}Ar, ^{14}C, ^{135}Cs, ^{3}H (tritium),

^{129}I, ^{81}Kr, ^{85}Kr, ^{40}K, ^{87}Ru, ^{79}Se, ^{90}Sr, ^{99}Tc and ^{126}Sn. Chemically toxic elements that have significant instant-release fractions are bromine, cesium, selenium and technetium. Instant-release fractions are associated only with the dissolution of the used-fuel matrix; there is no instant release for contaminants in the Zircaloy matrix.

We represent the two release mechanisms using different mathematical expressions:

- Congruent release is represented using a partial differential equation that describes the dissolution rate of the matrix material and the transport of a released contaminant through the buffer (Johnson et al. 1994b). The source boundary condition for the equation is a constant concentration given by the solubility of used-fuel pellets or Zircaloy. The outlet boundary condition assumes that the flux of a contaminant out of the buffer is proportional to its concentration at the outer edge of the buffer. The constant of proportionality is called the mass transfer coefficient of the waste matrix, and its value depends on the mass transport properties of the adjoining media (Garisto and LeNeveu 1989). Congruent release may also be modified by precipitation of the matrix material (Section 5.2.2.4).

- Instant release is represented by a partial differential equation that describes the diffusion of an instantly released contaminant out of the containers and buffer (Johnson et al. 1994b). The initial condition or source boundary for this equation depends on the initial concentration of a contaminant in the container and on rates of loss of the contaminant resulting from decay and diffusion. We assume that contaminant transport within the buffer is not affected by the properties of the surrounding rock or backfill.

These differential equations simulate the time-dependent release of contaminants from the waste matrices, starting when groundwater has corroded the container and contacted the waste.

5.2.2.2 Container Lifetimes

Most of the Grade-2 titanium containers are expected to last for at least 10^3 a (Johnson et al. 1994b) before they eventually fail through the corrosive action of the groundwater. The vault model contains a mathematical function that describes the rate of container failures in the vault, incorporating major modes of failure caused by initial fabrication defects, crevice corrosion and delayed hydride cracking. The latter two modes of failure depend on temperature (Johnson et al. 1994b):

- crevice corrosion is more important for containers subjected to high temperatures; whereas

- delayed hydride cracking is more important for containers that cool quickly, and it occurs after the container temperature drops below about 30°C.

The container failure function takes into account the variability in container temperature in different sectors in the vault, so that different sectors have different rates of container failure (Johnson et al. 1994b). Important parameters required to describe the rate of container failure are the corrosion allowance thickness of the container wall (equal to a fraction of its actual thickness), the rate of corrosion of titanium alloy, and the probability of early container failure resulting from manufacturing defects.

To account for the fact that container failures would occur over several thousand years, we modify the movement of contaminants released from a waste matrix by combining it with the container failure function in a convolution procedure. The convolution modifies the movement of contaminants leaving all waste matrices in the vault, both congruently and instantly released, in accordance with the failure rate of the waste containers.

These calculations simulate the time-dependent release of contaminants from the containers into the buffer layer surrounding the containers.

5.2.2.3 Contaminant Transport through the Buffer and Backfill

Contaminants leaving the container must move through the buffer because the container is completely surrounded by buffer. We allow for two options for subsequent contaminant movement. The contaminants may

- Pass through the backfill if the backfill is between the buffer and the fracture zone. This is the case for the 12 sectors shown in Figure 5-10. Groundwater movement in the rock to the left of and below LD1 tends to be very slow, and contaminants would tend to diffuse upwards toward LD1 and the surface (Davison et al. 1994b). To account for the fact that the backfill is not a continuous layer across the entire vault, we assume an effective thickness for the backfill: it is only 1.4 m compared with its actual thickness of 5.5 m. This assumption is discussed in detail in the primary reference for the vault model (Johnson et al. 1994b).

- Pass directly into the rock if the backfill is not between the buffer and the fracture zone. This situation occurs in studies for derived constraints (see Section 6.2), which include examination of cases in which we assume that there are rooms on both sides of fracture zone LD1. For the rooms to the right and above LD1, there is no backfill between the buffer and the fracture zone. Moreover, groundwater movement above LD1 and near the reference disposal vault tends to be directed downwards toward LD1 (Davison et al. 1994b). Therefore, for these rooms, we assume that contaminants travel through the buffer and into the surrounding rock toward LD1.

The transport of contaminants in the buffer and backfill is modelled using partial differential equations. The equations use the simplified geometry shown in Figure 5-9 and represent the movement of contaminants from one sector through adjacent planar layers of buffer and (if required) backfill of appropriate thickness and area (Johnson et al. 1994b). They also represent the process of sorption, by which the buffer and backfill materials retard the movement of contaminants. The solutions to these equations describe the time-dependent release of contaminants from the buffer and backfill (including the containers and waste matrices) to the rock surrounding the reference disposal vault.

To completely specify the equations, we must define the source and outlet boundary conditions. The source boundary condition is the time-dependent rate of arrival of a contaminant at the beginning of the layer. For the buffer layer, the rate of arrival of a contaminant is given by its calculated rate of release from the containers. For the backfill layer (if it is required), the rate of arrival of a contaminant is given by its calculated rate of release from the buffer. The condition at the outlet or boundary (at the end of the layer) is a mass transfer coefficient pertaining to the buffer or the backfill, and its value depends on the mass transport properties of the adjoining media (Garisto and LeNeveu, 1989). For the buffer layer, the adjoining media are the backfill and rock or just the rock if the backfill is not in the contaminant movement path. For the backfill layer, the adjoining medium is the rock. These mass transfer coefficients are important elements of the linkage between the vault and geosphere models (see Section 5.3).

Important parameters used to describe contaminant transport through the backfill and buffer are the contaminant capacity factors (which describe the amount of contaminants sorbed onto the buffer and backfill) and diffusion coefficients, the thicknesses of the buffer and backfill layers, and the groundwater velocities near and in the vault.

5.2.2.4 Chemical Precipitation in the Buffer

The vault model allows for the possibility of chemical precipitation and subsequent re-dissolution of contaminants as they move through the buffer. Some contaminants that have dissolved inside the container could precipitate as they migrate into the buffer region with its different chemical environment.

The chemical environment may change because of radiolysis, which could produce localized concentrations of reactive molecular species near the container. These molecular species could affect the solubility of some contaminants, notably those whose solubilities are strongly affected by electrochemical potential. We expect the electrochemical potential would be more oxidizing near the container. The outer boundary of this oxidized region is called the redox front, and we assume it lies within the buffer. To better describe the electrochemical environment in the buffer, we use two electrochemical potentials in the vault model: one characteristic of the surface of a container and the other (which is slightly less oxidizing) characteristic of the surrounding buffer (Johnson et al. 1994b).

To model precipitation and re-dissolution, we use the following sequence of steps for all elements (with a modification for uranium described below) (Johnson et al. 1994b):

- We first estimate solubility limits for five elements: plutonium, technetium, neptunium, thorium and uranium. The limits are computed at the two electrochemical potentials, and we use the smaller of the two computed limits because precipitation should occur at the region of smallest solubility. The limits have a range of possible values, because they are calculated from parameters that are described using PDFs.

  For all other elements, we use input parameters to represent solubility limits in the expected chemical environment of the buffer. Because they are uncertain, these solubility limits are specified using PDFs.

- We then calculate two release rates for each contaminant: one pertains to release from the buffer ignoring precipitation, and the other to release from the buffer if the contaminant were dissolving at its solubility limit. If this latter, constrained, release rate is smaller than the former, then precipitation of the contaminant within the buffer is indicated and an adjustment to its release rate is required. This step and the next are performed separately for each contaminant in the nuclear fuel waste. Thus different isotopes of the same element are treated separately, which simplifies the mathematics and leads to overestimates of the releases of these isotopes from the buffer.

- We adjust the release rate of the contaminant if the previous step indicates that precipitation would occur. This adjustment uses the solubility-constrained rate described above and will reduce the release rate of the contaminant. We also simulate the accumulation of the contaminant as a precipitate in the buffer using an ordinary differential equation (Johnson et al. 1994b). The equation includes the effects of radioactive decay and re-dissolution of the precipitate. Re-dissolution is described in a manner similar to that discussed above for congruent release, except that it uses the solubility limit of the element within the buffer.

A special condition applies for uranium (Johnson et al. 1994b). We assume that uranium dissolves at its calculated solubility limit, using the electrochemical potential at the surface of the container. If precipitation in the buffer is indicated (using the sequence of steps noted above), we simulate its accumulation and re-dissolution as in the preceding paragraph.

In addition, the precipitation of uranium will also affect the dissolution of the used-fuel matrix. Precipitation of uranium reduces the concentration of the used-fuel matrix material (uranium) in the water of the buffer and, therefore, enhances the dissolution of used fuel. Consequently, precipitation also enhances the congruent release of all embedded contaminants. This effect is simulated by modifying the mass transfer coefficient of the used-fuel matrix and by using a buffer thickness equal to the distance from the container to the point of precipitation in the buffer (Garisto and LeNeveu 1989). These modifications increase the rate of dissolution of the used-fuel matrix and subsequent release of all embedded contaminants.

Important parameters describing precipitation in the buffer are the element solubility limits. For plutonium, technetium, neptunium, thorium and uranium, the calculation of solubility limits includes parameters representing the electrochemical potential in the buffer and thermodynamic equilibrium constants. These calculations modify the estimated release of contaminants from the buffer and backfill and provide adjusted time-dependent release rates for any element that precipitates. If uranium precipitates, these calculations also adjust the release rates for all contaminants released from used fuel by congruent dissolution.

5.3 LINKAGE BETWEEN THE VAULT AND GEOSPHERE MODELS

The vault model describes the engineered barriers in the reference disposal vault; the geosphere model describes the rock surrounding the vault and extending to the surface environment. The linkage between the vault and geosphere models provides an integrated description of interactions between these two components of the waste disposal system. Information is passed from one model to the other, so that the combined models provide a consistent representation of the vault and geosphere for the reference disposal system.

The vault model estimates the release of contaminants from the buffer and backfill to the surrounding rock, for each of the vault sectors (Johnson et al. 1994b). The principal link between the vault and geosphere models is provided by

- The time-dependent movement of contaminants that are passed from each of the vault sectors to the transport network of the geosphere model.

Additional links between the vault and geosphere models are provided through two other types of parameters:

- *Characteristics of groundwater movement.* The geosphere model (Davison et al. 1994b) determines the direction and magnitude of groundwater movement through the adjacent rock and through the buffer and backfill for each vault sector. These velocities are used in the vault model, ensuring that groundwater movement is consistent between the two models.

- *Properties of the rock surrounding the vault.* The geosphere model (Davison et al. 1994b) provides parameters describing sorption, diffusion, dispersion, groundwater velocity, porosity, tortuosity, and other properties of the rock surrounding each vault sector. These parameters (discussed further in Section 5.4) are used to calculate the mass transfer coefficients mentioned in Section 5.2 (Johnson et al. 1994b). Thus the release from each vault sector is dependent in part on the properties of the rock surrounding the sector.

These latter two linkages are designed to ensure that the rate of release of contaminants from each vault sector is consistent with the properties of the adjoining geosphere region.

5.4 DESCRIPTION OF THE GEOSPHERE MODEL

This section describes the main features of the geosphere and geosphere model that are important for the postclosure assessment of the SYVAC scenarios for the reference disposal system. Further details are provided in the primary reference for the geosphere model (Davison et al. 1994b), including justification of the assumptions and data used by the model.

5.4.1 Description of the Geosphere

In the description of the vault model for the reference disposal system, we discussed an assumed fracture zone, LD1, which passes through the plane of the vault (Figures 5-5 and 5-6). Fracture zone LD1 is also represented in the geosphere and has been included so that we could examine its effects on the performance of the disposal system and because fracture zones are common features on the Canadian Shield. Similarly, we include a well in the geosphere because wells are found at many sites on the Canadian Shield.

The geosphere also contains other features that are characteristic of a disposal system that would be located in the Canadian Shield, such as highly weathered rock near the surface. However, the geochemical, geological and hydrogeological details of the model are based on a particular site to ensure that the data used in the assessment are realistic and self-consistent. As noted previously, we have taken information from the WRA, which has been extensively studied for more than a decade (Davison et al. 1994b).

The WRA covers an area of about 750 km^2 in southeastern Manitoba (Figure 5-11), including both the WL and the URL. A major portion of the rock in the area is part of the Lac du Bonnet batholith, a large granitic pluton. The rock at the surface is a weathered red granite intersected by a set of subvertical fractures, and the deeper rock is an unweathered and sparsely fractured grey granite. Surface elevations are 300 m above mean sea level in the southeast, grading to 250 m above mean sea level in the northwest. The Winnipeg River System, nearly surrounding the area, provides hydrogeological boundary conditions. This river, together with the set of interconnected fracture zones and the topography, controls the pattern of groundwater movement in the area. We believe that these physical conditions would not change substantially over at least the next 10^4 a, the time frame of concern for the postclosure assessment (Davison et al. 1994b).

We assume that the vault of the reference disposal system is located at a depth of 500 m and that its geological and hydrological setting is similar to that of the URL in the WRA. Figures 5-12 and 5-13 are cross sections of

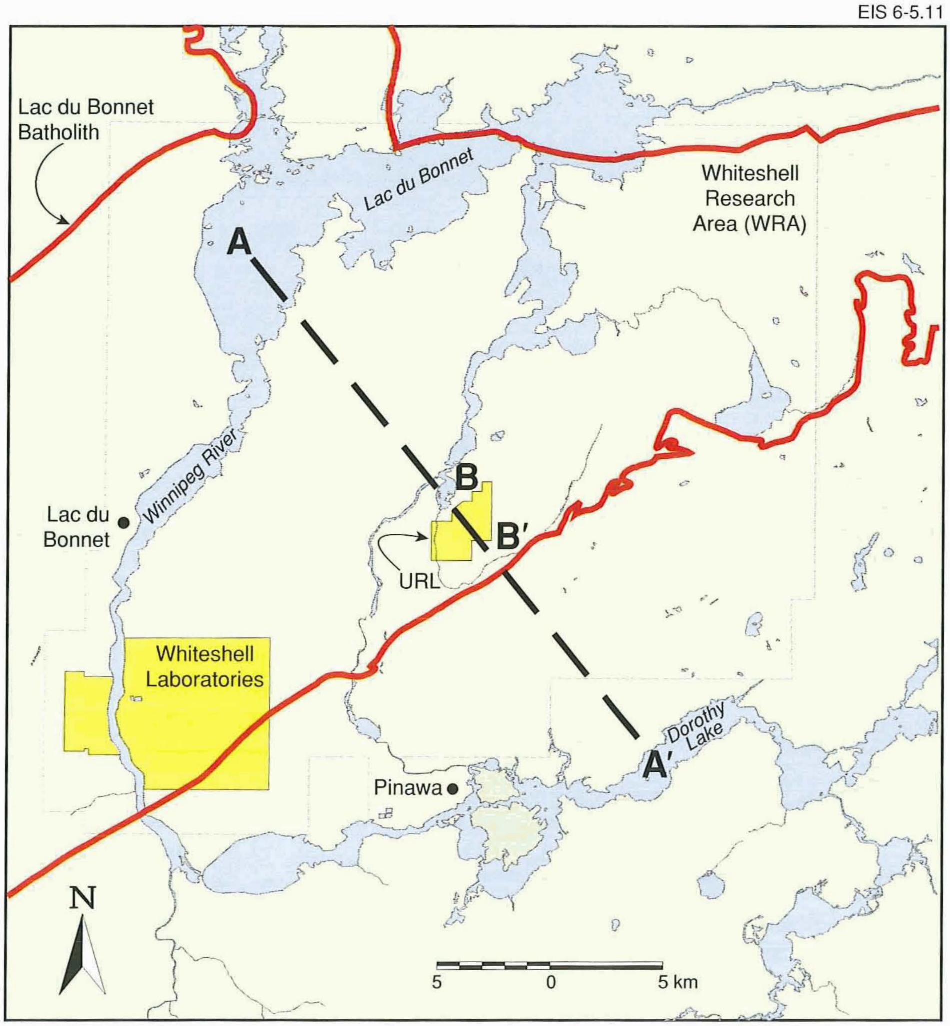

FIGURE 5-11: The Whiteshell Research Area

Shown is the location of the Underground Research Laboratory (URL), the Whiteshell Laboratories, and the townsites of Lac du Bonnet and Pinawa. The Winnipeg River nearly surrounds the study area. The dashed line, with labels AA' and BB', defines the location of the cross sections shown in Figures 5-12 and 5-13. The Lac du Bonnet batholith lies underneath most of the studied area. The WRA is used to model the regional groundwater flow regime and is described in the primary reference for the geosphere model (Davison et al. 1994b).

We have defined the reference disposal system on the assumption that its geological and hydrological characteristics are similar to those of this area.

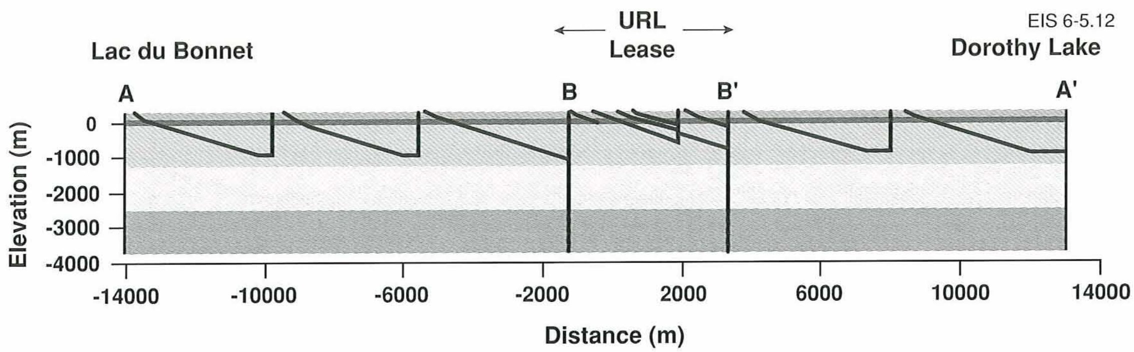

FIGURE 5-12: Vertical Cross Section Illustrating Geological Features of the Whiteshell Research Area

This section, along line A to A' of Figure 5-11, includes a pattern of known and assumed fracture zones (Davison et al. 1994b). We assume that some major vertical joints extend downwards to 4 km and correspond to components of the Winnipeg River System and the boundary of the Lac du Bonnet batholith. This figure also shows five different layers of bedrock, each with different hydrogeological properties. The upper two layers are relatively thin and represent the uppermost portion of highly weathered rock, and the less altered rock immediately below.
The region represented by this figure (and Figure 5-11) is used to model the regional groundwater flow regime (Davison et al. 1994b).

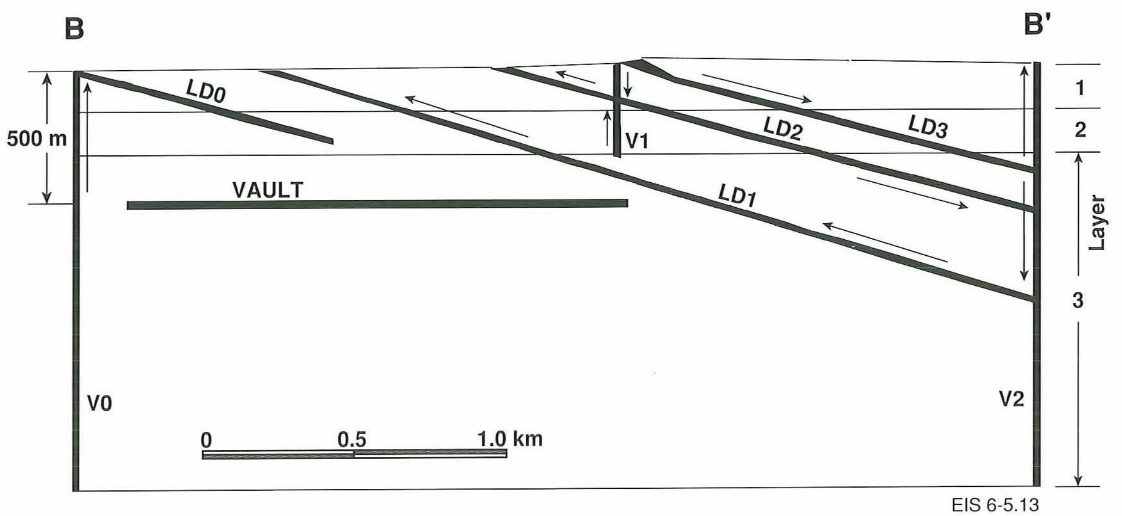

FIGURE 5-13: Vertical Cross Section of Known and Assumed Geological Features in the Vicinity of the Hypothetical Vault of the Reference Disposal System

This cross section is along line B to B' of Figure 5-11 and is based on observed and inferred geology near the Underground Research Laboratory; it includes low- dipping fracture zones (labelled LD0 to LD3) and vertical joints (V0 to V2) (Davison et al. 1994b).
In the postclosure assessment of the reference disposal system, we conservatively assume that fracture zone LD1 extends downwards, cutting through the plane of a hypothetical vault that is about 500 m below the surface. (LD1 is also discussed in the description of the vault model and in Figures 5-5 to 5-7.) The minimum distance from LD1 to the waste emplacement part of the nearest rooms is about 50 m and is referred to as the waste exclusion distance.
The fractures zones, vertical joints, and the topography control the direction and volume of groundwater movement in the geosphere and in the vicinity of the vault. Groundwater flow directions in fracture zones are indicated by the arrows. The overall tendency of groundwater movement is downward to LD1 on the right-hand side of the figure and upward along LD1 to the surface on the left-hand side. Groundwater movement is extremely slow in the sparsely fractured low-permeability rock near the vault.

part of the WRA, running from the northwest to the southeast. The cross section in Figure 5-12 represents an area about 4 km deep and 27 km wide. The regular pattern of fractures and joints is an extrapolation, based on data from the WRA and established geophysical principles (Davison et al. 1994b).

Figure 5-13 is an expansion, showing the location of the hypothetical vault and giving more detail of the nearby geological features. It shows four zones of low-dipping fractures and three vertical joints.
Because of their relatively high permeability, these features control the direction and volume of groundwater movement in the rock at the site (Davison et al. 1994b).

Current observations at the WRA show that fracture zone LD1 does not, in fact, extend to the depth of the hypothetical vault (Davison et al. 1994b). However, the hydrogeological information used in the postclosure assessment is based on information available in 1985, when a hydrological model of the WRA first became available (Davison et al. 1994b). At that time, the extent of fracture zone LD1 was uncertain and, to be conservative, we assumed that LD1 passes downwards through the plane of the disposal vault, that it is connected at depth to a vertical joint, and that the hydrological conditions allow for relatively rapid groundwater movement in the fracture zone. It is known that these assumptions lead to considerable overestimates of impact (Sections 6.3.3.5 and 6.6.2). We discuss in Section 8.2.6 how new information pertaining to LD1 would affect our results and conclusions.

For the assessment of the reference disposal system, the rock between the plane of LD1 and the nearest waste emplacement part of any vault room consists of about 50 m of sparsely fractured granite. This is the waste exclusion distance discussed in Section 5.2. Groundwater velocities within the rock of the waste exclusion distance are extremely small: the groundwater is essentially stagnant and, as discussed below and in Section D.3.1 in Appendix D, contaminant transport is dominated by diffusion and not by moving groundwater.

We also study cases where LD1 passes through the hypothetical vault. In developing derived constraints (see Section 6.2), vault rooms are also located above LD1, on the right-hand side of Figure 5-13. Groundwater movement in the rock near the rooms above and to the right of LD1 is substantially faster than movement in the rock near the rooms below and to the left of LD1.

More details on the geology and hydrology of the WRA are provided in the primary reference for the geosphere model (Davison et al. 1994b).

5.4.2 <u>Features of the Geosphere Model</u>

The mathematical representation of the geosphere, or geosphere model, is used to simulate the transport of contaminants in groundwater within the geosphere. It describes the processes in which contaminants that have been released from the vault pass through the surrounding rock and discharge into the biosphere. The model contains a network of pathways describing the groundwater movement within the geosphere, and we simulate the transport of contaminants through this network. The model is outlined below and discussed more fully in the primary reference for the geosphere model (Davison et al. 1994b).

5.4.2.1 Groundwater Movement within the Geosphere

A complete description of groundwater movement in the geosphere would typically involve a large region, such as that shown in Figures 5-11 and 5-12. In studies of groundwater movement at this scale, we assume that the only movement of water into the region is infiltration from rain and snow from above and from (in this case) the Winnipeg River System (Davison et al. 1994b). The only movement of water out of the region is at A in Figures 5-11 and 5-12, corresponding to the downstream end of the Winnipeg River. We also assume that there is no significant groundwater movement across the lower boundary of Figure 5-12, at a depth of 4 km (Davison et al. 1994b).

At the scale of Figure 5-12, groundwater movement is modelled using a computer code called MOTIF (Davison et al. 1994b). The weathered red granite at the surface is modelled as a homogeneous layer with a porosity of 0.005 and anisotropic permeabilities of about 10^{-15} m^2. The unweathered grey granite at the depth of the hypothetical vault (500 m) is modelled as a homogeneous layer with a porosity of 0.003 and an isotropic permeability of 10^{-19} m^2. Fracture zones are modelled as planar homogeneous zones with a uniform thickness of 20 m, a porosity of 0.10, and anisotropic permeabilities of about 10^{-13} m^2.

Results produced by MOTIF suggest that the movement of contaminants would be limited to a much smaller region than that shown in Figure 5-12. Consequently, for the postclosure assessment, we confine the simulation of groundwater movement and contaminant transport to the smaller region illustrated in Figure 5-13. We also model this smaller region with MOTIF using a finer level of detail. These latter studies (Davison et al. 1994b) are used to calculate the groundwater movement pattern through the rock:

- without the vault and without the well;

- with a hypothetical disposal vault located at a depth of 500 m near the location of the URL; and

- with the hypothetical vault and a well drawing different volumes of water from the fracture zone above the vault.

For a long-term assessment, a wide variety of well properties are possible, such as the depth and location of the well, its intended use, and whether there might be other wells nearby. The detailed studies using MOTIF examined a number of choices for well depth and location, and we have used these studies to define the following basic characteristics that would lead to overestimates of impact (Davison et al. 1994b).

- The well is located along the centre line (based on MOTIF calculations) of the plume of contaminated water that is moving up fracture zone LD1.

- If it is deep enough to extend through the overburden, we locate the well along this centre line so that it extends as deeply as possible into LD1. The depth of the well is sampled from a PDF based on current information on the depths of wells on the Canadian Shield (Davison et al. 1994b). We distinguish between two broad classifications of wells: overburden wells and bedrock wells. An overburden well is relatively shallow and extends only into the overburden above the rock of the geosphere. A bedrock well is generally deeper, and we conservatively assume that it always intersects fracture zone LD1 in the centre of the contaminant plume.

These characteristics are conservative because the well is located where it would potentially receive the greatest amounts of contaminants, and the choice of its depth and location provide for the shortest transport distance of contaminants from the vault. Moreover, contaminants from the vault are concentrated into a single well that serves as the sole source of drinking water for the critical group. (It may also be used to supply water for irrigation.)

The modelling of the well in the geosphere model includes the effects of water withdrawal on groundwater movement using an adjustable network of segments (see below) and modification to groundwater velocities in the affected segments. More features of the model for the well are discussed in the next two sections, describing the linkage between the geosphere and biosphere models and the biosphere model because its properties are affected by characteristics of both the geosphere and the biosphere.

For this postclosure assessment study, we simulate groundwater movement for the region around the hypothetical vault using a simpler transport network in a code called GEONET. The GEONET code uses results generated by MOTIF to describe the movement of the groundwater in a network of flow tubes or segments in the geosphere. That is, GEONET is calibrated against MOTIF, and it reproduces the pattern of groundwater movement and contaminant transport calculated by MOTIF (Davison et al. 1994b).

The segments of the transport network are selected to represent contaminant pathways through parts of the geosphere that have distinct chemical and physical properties (Davison et al. 1994b). For example, GEONET models the top three bedrock layers in Figure 5-12, and sets of segments are used to represent rock in each layer. The GEONET code also has other segments to represent the well and fracture zones, such as LD1 in Figure 5-13. These fracture zones, which actually consist of many interconnected fractures, are also modelled as homogeneous features with representative hydrological properties. The MOTIF code uses anisotropic permeabilities to account for the presence of fracturing in the different zones. Results from MOTIF are used to generate a transport network for GEONET in which the permeabilities are projected along the directions of the segments of the transport network (Davison et al. 1994b)). In general, the properties of the fracture zones and the surrounding rock are such that groundwater velocities are greatest (and subsequent contaminant transport is greatest) in the fracture zones that serve as preferential channels through the geosphere.

Segments connect to other segments at nodes. More precisely, the central flow line of a segment connects to the central flow line of an adjoining segment. We refer to a "central" flow line because each segment, or flow tube, represents a volume of rock with uniform properties, with contaminants entering and exiting at opposite ends (Davison et al. 1994b). There are 12 segments that originate at the 12 vault sectors and 4 segments that lead to each of the 4 discharge zones in the biosphere (Figure 5-14).

The following properties are assigned to the nodes: Cartesian coordinates and hydraulic heads. The following properties are assigned to segments: porosity, tortuosity, dispersivity, permeability, salinity of the groundwater, and the types and amounts of minerals affecting sorption of contaminants. All the properties are chosen to be consistent with results from MOTIF and with field and laboratory studies of the WRA (Davison et al. 1994b). The permeabilities, porosities and hydraulic heads are used to calculate the linear groundwater velocities along each segment, using Darcy's law. The groundwater velocities, dispersivities and tortuosities are used (with the free-water diffusion coefficients) to calculate dispersion coefficients. Salinities and mineralogies are used to calculate retardation factors (described further below). The primary reference for the geosphere model (Davison et al. 1994b) provides more information on these properties and the mathematical equations used in the calculations. Tables D-2 and D-3 in Appendix D list typical values for many of the parameters and calculated variables. They show that there is no significant groundwater movement in the rock surrounding the vault (the lower rock zone) so that contaminant transport in this region is dominated by diffusion.

The values for some of the above transport parameters are affected by the presence of a bedrock well, and the effects become more pronounced as more water is withdrawn from the well. We simulate these effects using analytical equations for a confined aquifer and empirical equations based on detailed results from MOTIF (Davison et al. 1994b). The equations

- adjust groundwater velocities in fracture zone LD1 leading to the well,

- adjust groundwater velocities in segments that lead from the vault to LD1,

- decrease volumes of groundwater produced at the other three discharge zones in the biosphere to correct for increased discharge from the well, and

- modify the diversion of contaminant movement into different segments to accommodate cases with small and large rates of withdrawal of water from the well.

A particularly important set of parameters in GEONET describes the transport network itself, defining how the segments are connected together, to form the set of contaminant pathways in the geosphere (Davison et al. 1994b). The important parameters required to describe the well are noted in Section 5.5.

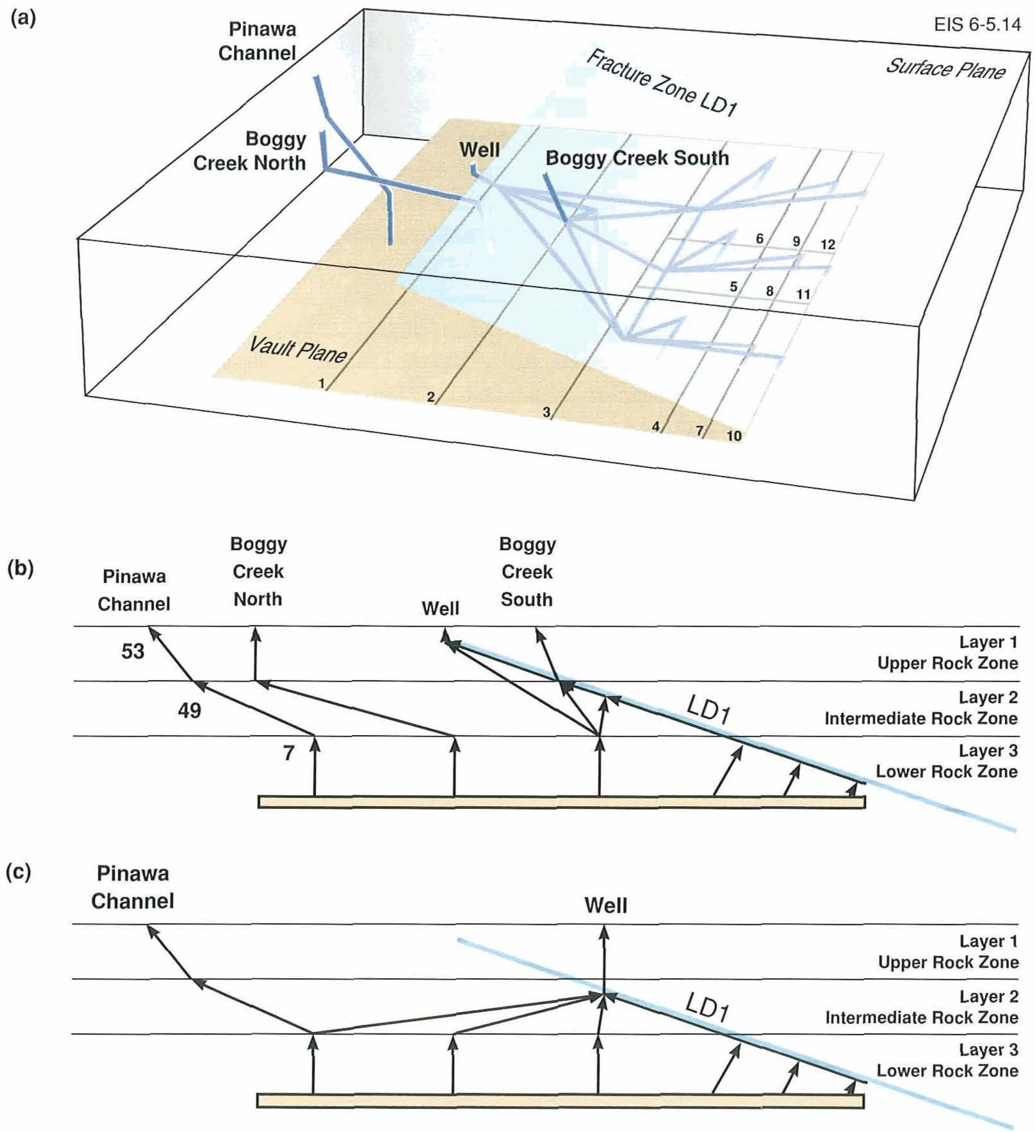

FIGURE 5-14: The Network of Segments Used by GEONET for the Reference Disposal System

Parts (a) and (b) apply to the case with small to moderate rates of withdrawal of water from a shallow bedrock well. Part (c) applies to the limiting case where withdrawal rates are large and from a deep bedrock well.

- Part (a) illustrates the set of segments leading from 12 vault sectors to 4 discharge locations in the biosphere. The shaded structure extending upwards from the lower right-hand corner represents fracture zone LD1. Segments within LD1 converge to discharge into Boggy Creek South and the well.
- Parts (b) and (c) are cross sections with projections of the transport network. The arrows indicate the direction of contaminant transport; for example contaminants leaving vault sector 1 travel along the segments numbered 7, 49 and 53, and end at the discharge location labelled Pinawa Channel. Contaminants released from other vault sectors discharge into Boggy Creek North, Boggy Creek South or the well.

The well receives more of the contaminants in part (c). In this limiting case of large rates of water withdrawal, the figure shows that contaminants no longer discharge to Boggy Creek North or Boggy Creek South, and that some contaminants are diverted to the well from the discharge at Pinawa Channel. There is a gradual diversion of contaminant movement from the set of segments shown in part (b) to those shown in part (c), depending on the rate of water withdrawal from the well.
The complete transport network used by GEONET to represent the reference disposal system has 46 segments, with 16 used to describe transport along LD1 (Davison et al. 1994b).

Another important parameter in the geosphere model is the groundwater velocity scaling factor. This parameter describes the uncertainty in groundwater velocities in the transport network. Groundwater velocities are correlated, so that if the velocity in one segment were to increase, then so must the velocity in all segments connected to it. For the postclosure assessment, we assume that the velocity scaling factor can be applied uniformly to all segments. This simple representation has two important features:

- It leads to a simple model of the geosphere containing the information from MOTIF relevant to contaminant transport from the vault. In particular, a simulation using a velocity scaling factor of unity simulates the groundwater movement calculated by MOTIF for present day conditions.

- It ensures that neither accumulation nor loss of groundwater will occur anywhere in the transport network.

5.4.2.2 Contaminant Movement through the Geosphere

Each segment is part of one or more pathways for movement of contaminants in groundwater from the vault to the biosphere. The 12 segments that originate at the 12 vault sectors eventually lead to 4 nodes representing discharge zones in the biosphere (labelled as Pinawa Channel, Boggy Creek North, Boggy Creek South and the well in Figure 5-14).

Figure 5-14 illustrates the network of pathways used in representing the reference disposal system. The pathways are represented by chains of segments in the geosphere model (Davison et al. 1994b). For example, the segments numbered 7, 49 and 53 in Figure 5-14b lead from vault sector 1 (the locations of the vault sectors are shown in Figure 5-10). Figure 5-14b indicates that contaminants released from vault sector 1, if they do not decay beforehand, would eventually reach the biosphere at the discharge zone labelled "Pinawa Channel"; contaminants released from vault sector 2 would eventually reach "Boggy Creek North"; and contaminants released from sectors 3 to 12 on the right-hand side of the vault would discharge at "Boggy Creek South" or the "well." The four discharge zones simulated in the geosphere model are shown in Figure 5-15.

Figure 5-14 shows that there are more vault sectors and geosphere segments near the fracture zone. To simulate the SYVAC scenarios for the reference disposal system, GEONET uses a total of 46 segments in the entire transport network, including 16 to simulate contaminant movement in fracture zone LD1 (Davison et al. 1994b).

Part (a) of Figure 5-14 is a three-dimensional representation, and parts (b) and (c) are cross sections showing projections of the transport network. Parts (a) and (b) exhibit the transport network followed by moving contaminants for small rates of withdrawal of water from a shallow well. Part (c) is the limiting network followed by moving contaminants when the withdrawal rate is large and from a deep well. (This change in the segments of the network is the modification referred to in Section 4.1.4, which allows the high-demand well scenario to be included within the SYVAC

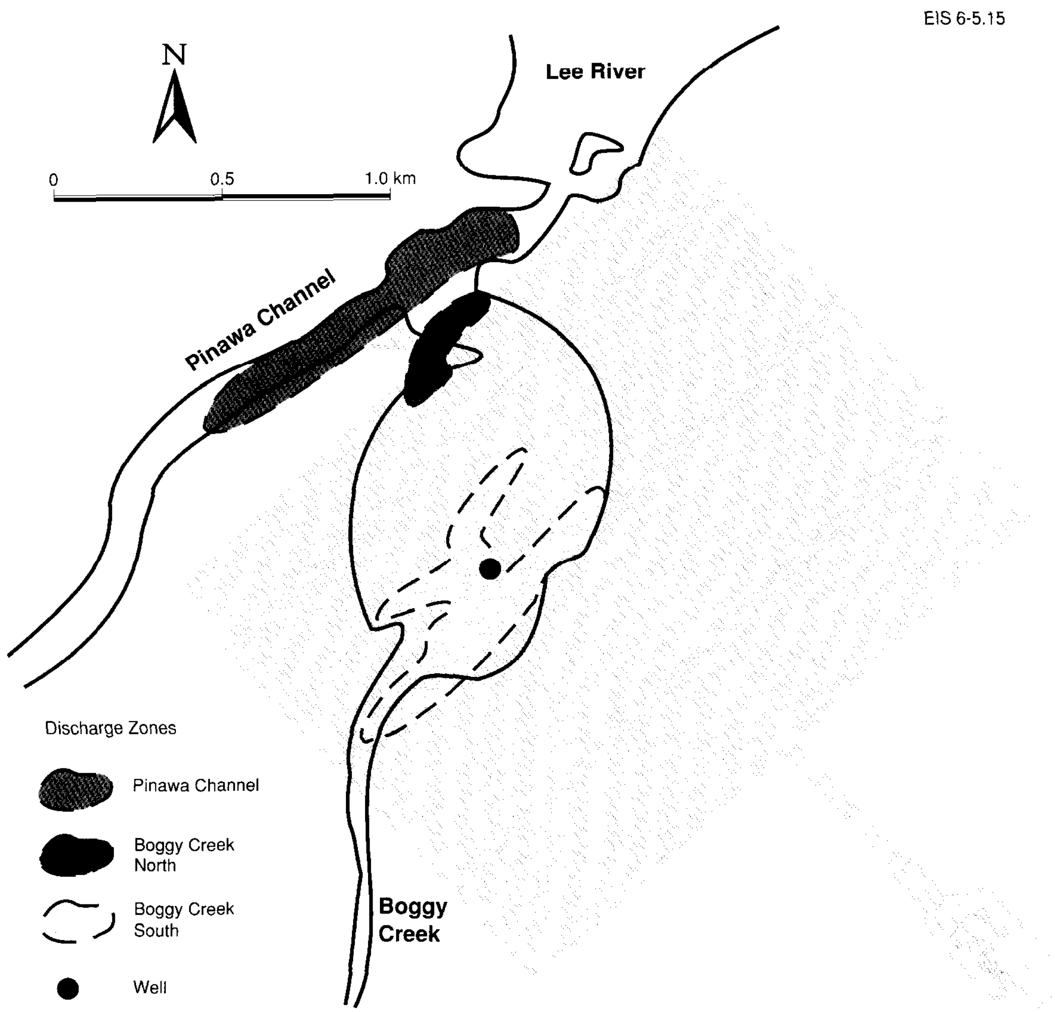

FIGURE 5-15: Discharge Zones in the Biosphere for the Reference Disposal System

The network of geosphere segments reaches the biosphere at four locations: Pinawa Channel, Boggy Creek South, Boggy Creek North and the well. The first three discharge zones are water bodies and wetlands in topographic lows.

We assume that the location of the well is constrained to lie along the centre of the contaminant plume moving up fracture zone LD1. The centre of this plume is offset from the centre line of the vault because of the direction of prevailing groundwater movement. Different well depths are modelled, with two general classes of wells: overburden and bedrock wells. We assume that overburden wells are relatively shallow and do not extend past the overburden overlying the rock of the geosphere. Bedrock wells are deeper, and we assume they are located such that they would intersect and draw water from LD1 as far down in the geosphere as possible. This figure and Figure 5-14 illustrate cases involving bedrock wells.

In this figure, the depth of the (bedrock) well is 37 m. For this depth, and with the constraint mentioned above, the well would lie within the current confines of Boggy Creek. This situation could occur sometime in the future if parts of Boggy Creek become filled with sediment or if water levels fall. We have assumed the constraint on the well location (along the centre of the contaminant plume) so as to overestimate subsequent estimates of dose.

scenarios for the reference disposal system.) The geosphere model includes both sets of segments to accommodate different amounts of withdrawal of water. A gradual diversion of contaminant movement is made from one set of segments to the other as the well demand changes. At intermediate well demands, both sets of segments constitute potential pathways for contaminant transport.

We simulate the movement of contaminants from the vault to the biosphere along these networks of segments. Contaminant movement is described mathematically using partial differential equations (Heinrich 1984b, Davison et al. 1994b). The equations describe contaminant transport by moving groundwater, dispersion and diffusion, and contaminant sorption onto minerals present in each segment. The equations also describe the increase and loss of contaminant masses resulting from radioactive decay. As for the vault model, we specify source and outlet boundary conditions for the equations:

- For the 12 segments adjoining the vault, the source boundary conditions are the time-dependent release rates of contaminants generated by the vault model. For all other segments, they are the time-dependent rates of arrival of contaminants from segments closer to the vault.

- The outlet boundary conditions assume that contaminant transport within each segment is not affected by the properties of any following segments or the discharge locations in the biosphere.

Important parameters used to describe the rate of contaminant transport in each segment include the properties of the segment, such as permeability, porosity and groundwater velocity. Free-water diffusion coefficients for the different contaminants and the tortuosity associated with a segment are also required to describe contaminant transport by diffusion in pore water.

An additional set of parameters is used to describe the extent of sorption of each contaminant on the minerals present in a segment. These sorption parameters, together with the types and amounts of minerals in a segment, are used to calculate a retardation factor for that segment (Davison et al. 1994b). The retardation factor is equivalent to the ratio of the groundwater velocity to the contaminant transport velocity. Its minimum value is unity, in which case the contaminant moves at the same velocity as the groundwater. A value greater than unity means that the migration velocity of the contaminant is slower than that of the groundwater; that is, the movement of the contaminant is retarded relative to the movement of the groundwater. (Table D-2 in Appendix D lists typical values of the retardation factor for many elements.)

5.5 LINKAGE BETWEEN THE GEOSPHERE AND BIOSPHERE MODELS

The geosphere model describes the rock surrounding the reference disposal vault and extending to the surface environment, and the biosphere model describes this surface environment, including humans and biota that live in the vicinity. The linkage between the geosphere and biosphere models provides an integrated description of interactions between these two components of the waste disposal system. It is composed of the information that is passed from one model to the other, so that the combined models provide a consistent representation of the geosphere and biosphere for the reference disposal system.

The geosphere model estimates the release of contaminants and the movement of water from the geosphere to four discharge zones in the biosphere illustrated in Figure 5-15 (Davison et al. 1994b). The principal link between the geosphere and biosphere models is

- the time-dependent movement of contaminants ending at the four locations of discharge.

Other linkages between the two models are described in the following paragraphs.

Three of the geosphere discharge zones are to bodies of surface water and wetlands in topographic lows. Related information passed from the geosphere model to the biosphere model is as follows.

- Contaminants reaching these three discharge zones must pass through a layer of overburden and a layer of compacted sediment, which are located between the last geosphere segments in the pluton and each of the three surface water discharges. (The three discharge zones include aquatic and terrestrial areas. Discharges to the aquatic areas pass through the overburden and compacted sediment, whereas discharges to the terrestrial areas pass through only the overburden (Davis et al. 1993)). These layers are too small to be represented in the detailed modelling using MOTIF (Davison et al. 1994b), but they are an important part of the pathways for groundwater and contaminants. We simulate their effects by adding six segments to the GEONET network (Davison et al. 1994b), one representing overburden and one representing compacted sediment for each of the three surface water discharge areas. We choose parameters describing these additional segments from field data, with the direction and magnitude of groundwater movement consistent with the results from MOTIF.

- The time-dependent movement rates of contaminants leaving the compacted-sediment layers are passed to the lake water modelled in the biosphere model. We also assume that some of the contaminants leaving the overburden layer directly contaminate the soil on the nearby banks of the water bodies, below the level of the water table. This feature is described by a parameter that estimates the fraction of contaminated groundwater that reaches the soil (Davis et al. 1993).

The fourth geosphere discharge zone is the well. Related information passed between the geosphere and biosphere models is as follows:

- We must ensure that the well can supply the amount of water that is to be withdrawn. The flow capacity of the well is calculated in the geosphere model, based on an equation that considers the depth and location of the well and the physical properties of the geosphere zone from which the water is drawn (Davison et al. 1994b). This flow capacity is then compared with a tentative *well demand*, or the amount of water desired from the well for use by the critical group, which is calculated in the biosphere model (Davis et al. 1993). If the tentative well demand exceeds the well flow capacity, we assume that the critical group uses both the well and the lake as sources of water: typically, the group would then obtain their domestic water from the well and their irrigation water from the lake (Davis et al. 1993). In this manner, the tentative well demand is sufficiently decreased so that it does not exceed well capacity. The resulting adjusted well demand is then used in the geosphere model for calculation of properties affected by the presence of the well and for estimation of contaminant concentrations in well water.

- In most simulations, the flow of water into the well includes some water captured from the surface; we assume that this surface water is contaminated to the same degree as the lake water. Surface water is captured by the well when (Davison et al. 1994b) the well demand is sufficiently large to depress the water table around the well, so that surface water flows to the well (this feature is a function of the depth of the well); or when the well is relatively shallow (not deeper than the thickness of the overburden), in which case we assume that the flow of water into the well is entirely from the surface water (and has contaminant concentrations equal to that in the lake water).

Important parameters used to describe the well are the depth and location of the well, related properties in the geosphere, and (from the biosphere model) the well demand and concentrations of contaminants in the surface water and in the well water.

Some additional parameters are passed from the geosphere model to the biosphere model to ensure that the models are consistent. These parameters are (Davison et al. 1994b, Davis et al. 1993)

- the areas of the three discharge zones located in topographic lows, shown in Figure 5-15;

- the volumes of groundwater reaching these three discharge zones; and

- contaminant sorption coefficients in the overburden layers and retardation factors in the compacted-sediment layers at the three discharge zones.

5.6 *DESCRIPTION OF THE BIOSPHERE MODEL*

This section describes the main features of the biosphere and biosphere model that are important for the postclosure assessment of the SYVAC scenarios for the reference disposal system. Further details, including justification of the assumptions and the data used by the model, are provided in the primary reference for the biosphere model (Davis et al. 1993) and in its four supporting reports (Amiro 1992b, Bird et al. 1992, Sheppard 1992, Zach and Sheppard 1992).

5.6.1 Description of the Biosphere

For the postclosure assessment of the reference disposal system, the local biosphere has the characteristics of the Shield region of central Canada. Figure 5-16 illustrates its key physical elements:

- the surface water body consisting of a lake and the mixed sediment on the lake bottom;
- a well that may supply the critical group with domestic and irrigation water;
- the soils in nearby cultivated and natural areas (the garden, forage field, woodlot and peat bog that supply the critical group with food, fuel and building materials and that serve as the habitat for native wildlife and plants); and
- the atmosphere above the lake and fields and inside buildings.

The biological features of the biosphere model are also designed to be typical of the Shield region in central Canada. That is, the assumed characteristics of plants, animals and other forms of life that are significant for the assessment are those that are typical of flora and fauna in the Shield region (Davis et al. 1993).

Another important element of the biosphere is the people who would be affected by the disposal facility. We use the concept of a critical group, consistent with AECB criteria (1987a). It is defined as follows (Davis et al. 1993):

- The critical group is the hypothetical group of individuals expected to receive the largest annual effective dose equivalent from the reference disposal facility.

  In this report, we use the abbreviation "annual dose" to mean "annual effective dose equivalent." Both represent the sum, over one year, of the effective dose equivalent resulting from external exposure and the 50-year committed effective dose equivalent from that year's intake of radionuclides (Davis et al. 1993). They determine the estimated biological consequences of internal and external exposures, with corrections accounting for the effectiveness of different types of radiation in causing biological damage and the radiosensitivity of different body organs. The qualifier "50-year committed" means that internal exposure includes the dose received during the current year, plus the dose that would be received over the next 49 years from those radionuclides that may remain in the human body.

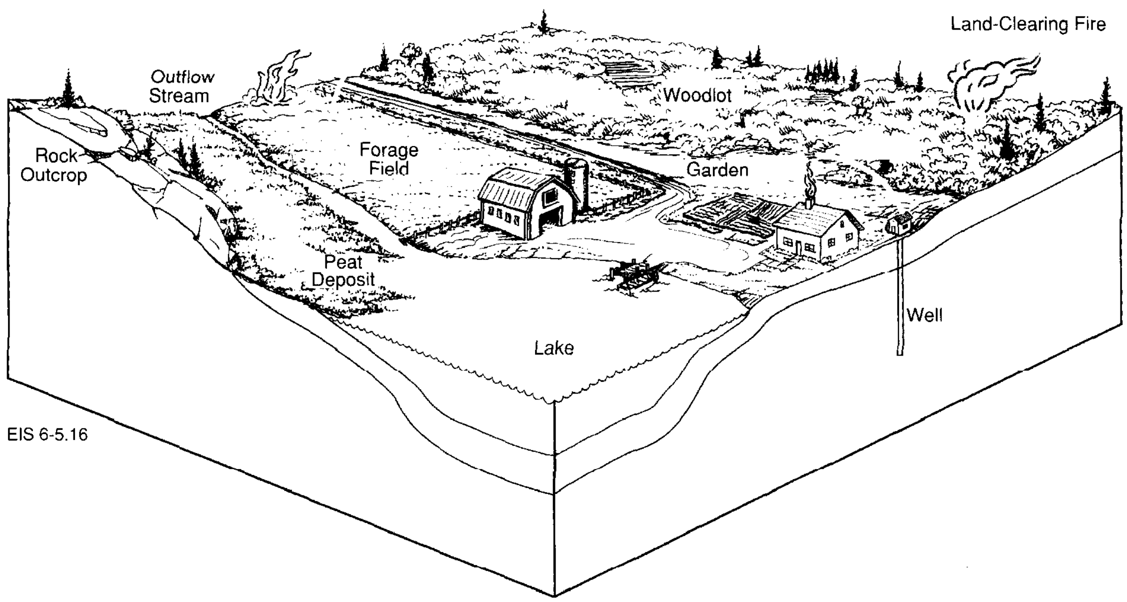

FIGURE 5-16: Key Elements of the Biosphere

The modelled biosphere includes a lake with lake sediment; a well that may serve as a source of domestic and irrigation water; soils in a garden, a forage field, a woodlot and a peat bog; and the atmosphere above the lake and fields. Discharges from the disposal vault are to the well and to three zones that underlie portions of the lake bed and the fields bordering the lake. We assume that members of the critical group spend all their lives in the area.

For the postclosure assessment, we make some assumptions on the characteristics of the critical group to ensure that radiation doses received are the largest (Davis et al. 1993). One such assumption is that its individuals spend all their lives in the area near the four discharge zones. We also assume that a succession of such groups permanently occupies the area. Every group obtains all its food, water, fuel and building materials from the contaminated zone. The food includes plants grown in a garden and wild berries, domesticated and game animals, upland birds and water fowl, dairy and poultry products, and fish from the lake. The domestic and irrigation water supplies come either from the nearby lake or from a well located above the disposal vault. This lifestyle is consistent with, but more self-sufficient than, current habits and will lead to overestimates of impacts.

We also consider potential effects to nonhuman biota in the biosphere model. Four generic target organisms are examined: a bird, mammal, fish and plant.

To the extent possible, we describe a generic biosphere that is representative of the Shield region of central Canada. Where necessary, we have limited some of its characteristics to match the actual surface environment of the WRA to ensure that there is a consistent relationship between the biosphere and its underlying geosphere.

One such limitation applies to the connection between the biosphere and geosphere models. In the description of the geosphere model and its linkage to the biosphere model (Section 5.5), we note that contaminants from the vault reach the biosphere at four discharge zones: three to surface waters and wetlands in topographical lows (with a small terrestrial component), and the fourth to the well (Figures 5-15 and 5-17). We have selected the characteristics of these discharge locations to be consistent with the geology, topography and climate of the WRA (Davis et al. 1993).

These characteristics include the size of the lake (the lake is assumed to be the body of water labelled Boggy Creek (Davis et al. 1993)), the size of the watershed that feeds the lake, and the annual precipitation.

These limitations do not unduly restrict the utility of the biosphere model. Most discharge locations in the Canadian Shield would also involve water bodies, wetlands and wells, similar to the discharges included in the biosphere described in the postclosure assessment. In addition, other characteristics of the biosphere model have been selected to be representative of a wider range of potential sites on the Canadian Shield (Davis et al. 1993).

5.6.2 Features of the Biosphere Model

The mathematical description, or model, of the biosphere is used to simulate the transport in the surface environment of contaminants that have arrived from the geosphere. It describes quantitatively the processes identified as important in estimating the movement of contaminants and subsequent effects on members of the critical group and other biota.

We assume one simplification throughout the biosphere model: the climate remains in an interglacial phase of the glaciation cycle, with conditions much as they are at present (Davis et al. 1993). This ensures that a thriving biological system, including humans, can be supported at the site at the time the effects are to be estimated. Some implications of glaciation are discussed in the primary reference for the biosphere model (Davis et al. 1993).

We describe the biosphere using several interconnected submodels. Figure 5-18 presents an overview of the interconnections among the four submodels (or component models) that make up the biosphere model: the surface water (lake water including mixed sediment), soil, atmosphere, and food-chain and dose (internal and external dose pathways) models. Not

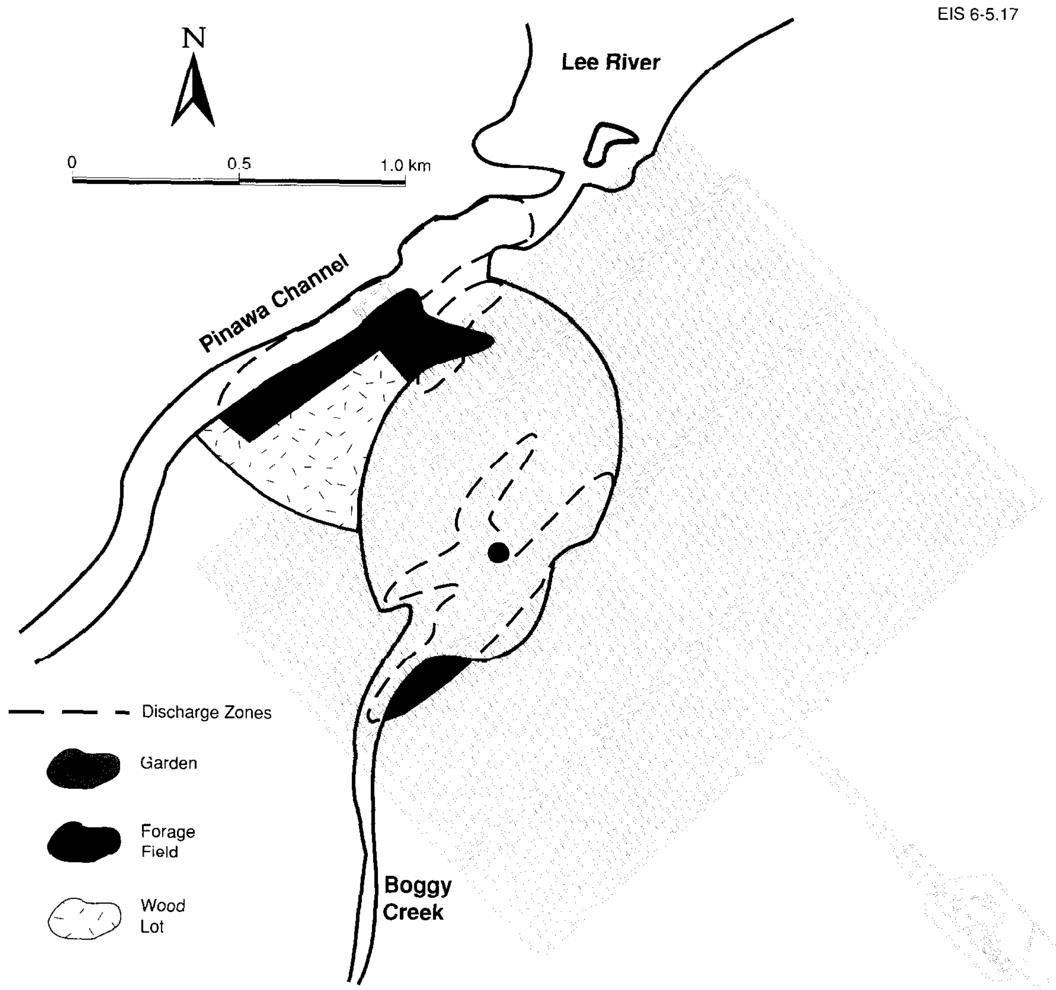

FIGURE 5-17: Plan View of the Surface Environment of Part of the Whiteshell Research Area

We have defined the reference disposal system using specific information on the biosphere near the WRA and more general information from the literature. For this system, contaminants from the geosphere enter the biosphere at four discharge zones (Davison et al. 1994b). Three are topographic lows: Pinawa Channel, Boggy Creek South and Boggy Creek North, and the fourth is the well. The garden, forage field, wood lot and peat bog used by the critical group are located within or near the discharges to the three topographic lows. We first locate the garden in the most-contaminated discharge zone; then the forage field in the remaining most-contaminated zone, and so forth.

This figure shows the location of the well when its depth is 37 m: it lies within the current confines of Boggy Creek. This unusual situation arises so that we would obtain overestimates of subsequent dose, by constraining the well to lie along the centre of the contaminant plume that is moving up fracture zone LD1 and at a location where the well intersects LD1 as far down in the geosphere as possible (Davison et al. 1994b). Although it is unrealistic today, in the future parts of Boggy Creek may become filled with sediment.

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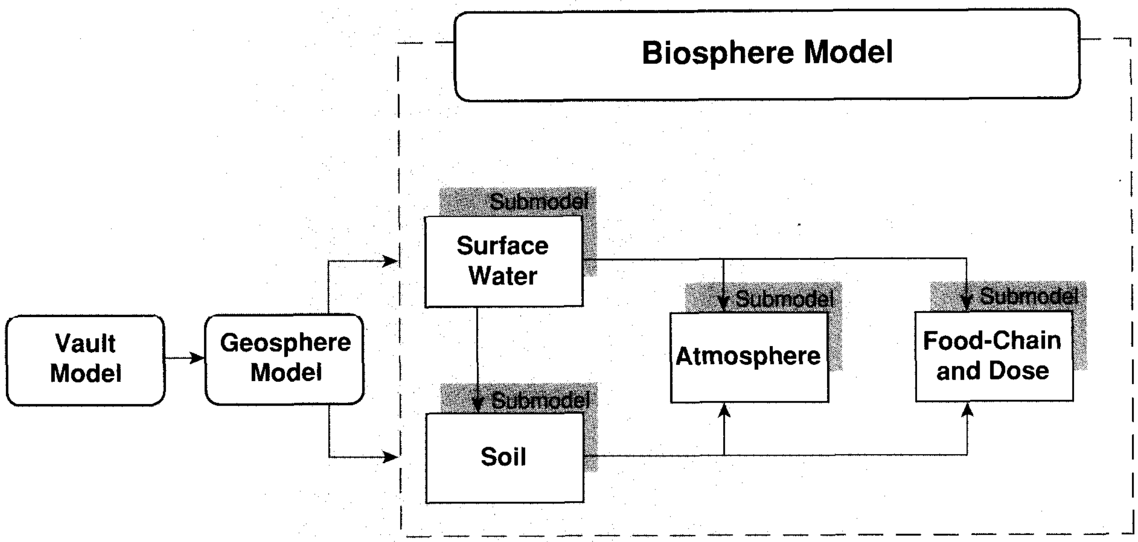

FIGURE 5-18: Interconnections Among the Four Component Models That Make up the Biosphere Model

This figure is considerably simplified; in general, each of the biosphere component models are joined to all others by many connections (see Figure 5-3 and Davis et al. 1993). Contaminants from the vault pass through the geosphere and enter the biosphere at aqueous and terrestrial discharge locations. These discharge locations are described by models for the surface water body (a lake and lake sediment) and soil. Transport within the biosphere is described using the surface water, soil, atmosphere, and food-chain and dose models. The latter model also simulates internal and external dose pathways. Not shown is the model for the well, which is part of the linkage between the geosphere and biosphere models (Section 5.5). Contaminants from the geosphere that enter the well are also passed to the surface water, soil, atmosphere, and food-chain and dose models.

We use the biosphere model to simulate transport between the parts of the biosphere and to calculate concentrations of contaminants in the lake and lake sediment, well, soil, and atmosphere used by members of the critical group. For radioactive contaminants, we also estimate annual doses to members of the critical group and to other organisms.

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shown in this figurc is thc model for the well, which is described in Section 5.5 as part of the linkage between the geosphere and biosphere models. Contaminants from the geosphere that enter the well are also passed to the surface water, soil, atmosphere, and food-chain and dose models. In general, the interconnections are more complex than those illustrated: each of the submodels is joined to all others by one or more connections (Davis et al. 1993).

Contaminants arriving from the geosphere may enter the biosphere via the well, lake sediment and soil, and subsequently spread to the atmosphere.

However, we assume that all flows from the geosphere eventually reach the surface water (except for the noble gases, which we assume discharge from the geosphere directly into the surrounding atmosphere where they may result in radiation doses resulting from external exposure (Davis et al. 1993)). In fact, we satisfy this assumption in a conservative manner, by duplicating the mass of contaminants. For example, at any point in time the mass of ^{129}I discharged to the well and to all the terrestrial discharge areas is also assumed to exist in the lake (this topic is discussed further in the description of the surface water model). Algebraic equations are used to estimate concentrations of radionuclides in the food chain (except the noble gases) and to calculate the total annual dose (internal and external) to a member of the critical group (Davis et al. 1993). Total annual dose is also estimated for other biota. For chemically toxic elements, concentrations are estimated in the water, air and soil used by members of the critical group.

We simulate the movement of contaminants in each part of the biosphere using ordinary differential equations or algebraic expressions that describe the movement of contaminants (Davis et al. 1993). The equations include expressions to account for the following processes:

- Transport of contaminants within each part of the biosphere. For example, the equations for the soil describe the movement of contaminants from the soil near the water table to the plant rooting zone.

- Transport of contaminants between parts of the biosphere. For example, a set of equations accounts for the transfer of contaminants from lake water and soils to the atmosphere through suspension of contaminated particulates and degassing of volatile contaminants. (For carbon, the parameters are called the gaseous evasion rates from soil and from the lake; for iodine, they are the gaseous evasion rate from soil and the aquatic mass loading coefficient from the lake (Davis et al. 1993).)

- The loss of a radionuclide because of its radioactive decay and the gain due to the decay of a precursor radionuclide. (We do not simulate radioactive decay in the atmosphere because we assume that the effects of decay are unimportant over the short time-scales of other processes involved (Davis et al. 1993).)

Several parameters are common to more than one part of the biosphere, so that the modelling of related processes is consistent. Two examples of common parameters are:

- *Source of water used by the critical group.* The critical group obtains its water (for household use and for watering the garden) from a well or a lake, and the source of water determines the subsequent contaminant movement from the well or lake to other parts of the biosphere.

- *Number of persons in the household of the critical group, or size of the critical group.* The number of individuals in the critical group affects the sizes of the fields (garden, forage field, woodlot and peat bog) and the volume of water withdrawn from the well or lake.

In the following paragraphs, we outline the processes that are simulated in each component of the biosphere model and list important parameters. More detail on the biosphere model and data is provided in the primary reference for the biosphere model (Davis et al. 1993).

5.6.2.1 Surface Water Model

The surface water body or lake includes the body of water called Boggy Creek in Figure 5-15 (Davis et al. 1993). It is the site of the processes illustrated in Figure 5-19. Some of these processes also appear in Figure 5-20 for the soil model. We model it as a well mixed, constant-volume water body fed by runoff from the watershed (Bird et al. 1992). Mixed sediment is continuously being deposited on the lake bottom, removing contaminated material from the lake water above. The contaminants lost from the lake water to the mixed sediment are still accessible to the critical group because mixed sediment may be used for field soil or as a source of inorganic building materials (such as sand and aggregate).

We describe the transport of contaminants in the lake and mixed lake sediment using ordinary differential equations containing rate terms representing the movement of contaminants to and from the water and sediment and between the water and sediment (Bird et al. 1992, Davis et al. 1993). We assume all contaminants released from the geosphere eventually enter the lake. Thus the lake and lake sediment receive contaminants

- from the groundwaters discharged from the geosphere, rising through a deep layer of compacted sediment and arriving at the aquatic and terrestrial parts of the discharge zone; and

- from any contaminated water that has been drawn from the well.

Upon reaching the lake, we assume that the contaminants are rapidly and uniformly dispersed throughout its volume. Contaminants may leave the lake water by

- the use of lake water to supply household water and irrigation water required by the critical group,

- suspension of contaminated particulates to the atmosphere,

- degassing of volatile contaminants to the atmosphere,

- radioactive decay,

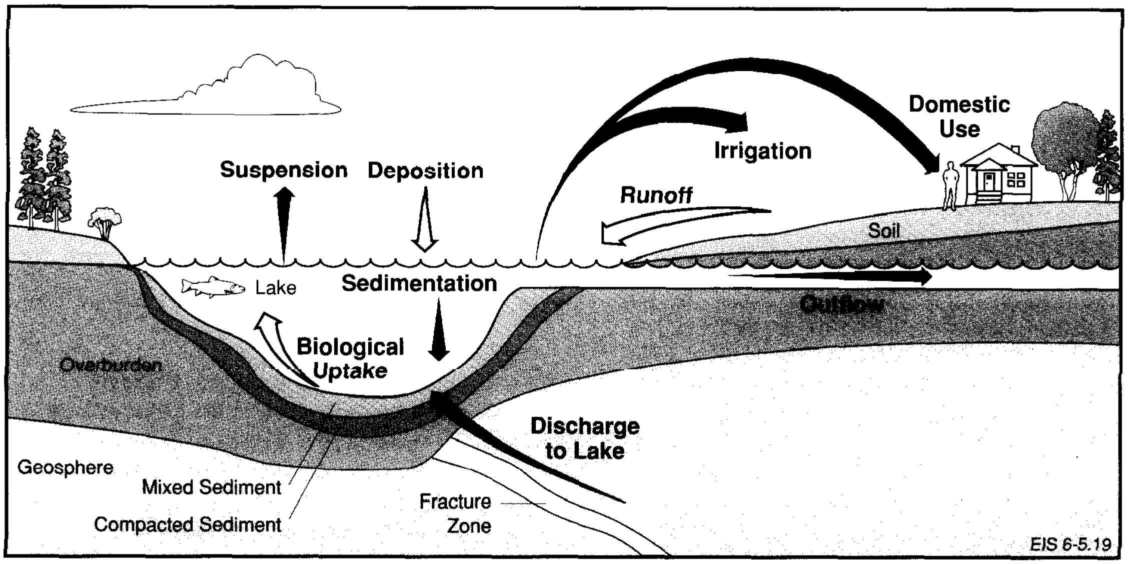

FIGURE 5-19: The Processes Modelled in the Lake and Lake Sediments Model

The solid arrows show processes that are explicitly modelled in the surface water model and the open arrows indicate processes that are implicitly considered (Davis et al. 1993). The primary sources of contaminants are the well (not shown) and groundwater discharging through the overburden to the compacted sediments (these sediments underlie Pinawa Channel and Boggy Creek shown in Figure 5-16). Contaminants leave the lake water by radioactive decay (not illustrated), particle suspension and degassing to the atmosphere, sedimentation to the mixed sediments, pumping for domestic and irrigation use by the critical group, and outflow downstream. We assume that all contaminants eventually return to the lake, except those lost by radioactive decay, outflow, and (for ^{14}C and the noble gases) by degassing.

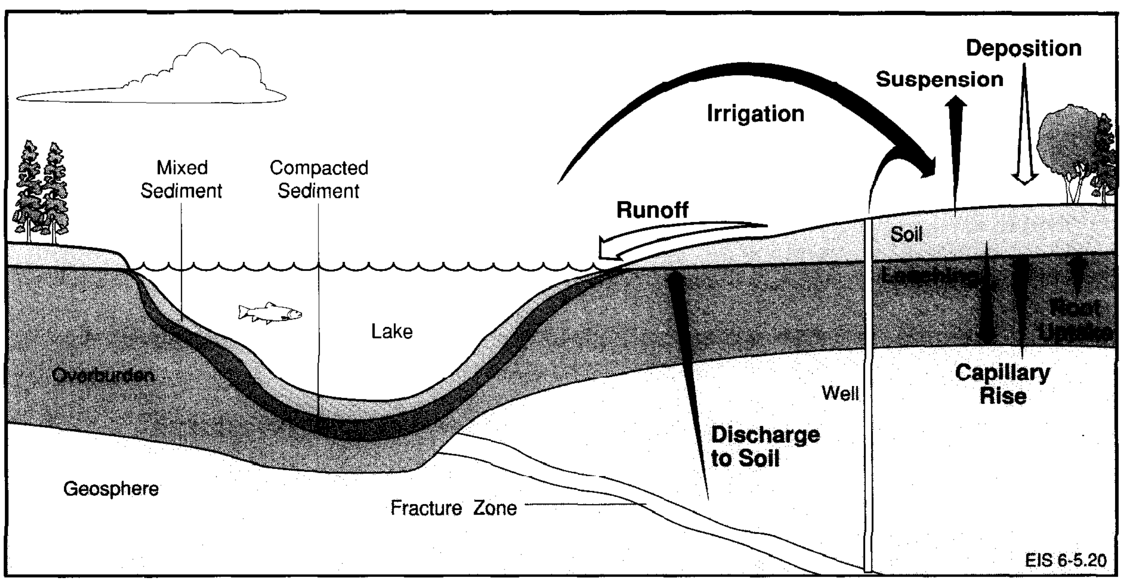

FIGURE 5-20: The Processes Modelled in the Soil Model

The solid arrows show processes that are explicitly modelled in the soil model, and the open arrows indicate processes that are implicitly considered (Davis et al. 1993). Four fields are modelled in a similar manner: a garden, a forage field, a woodlot and a peat bog (shown in Figure 5-16). Contaminants enter each field by capillary rise from the water table below the soil, by air deposition of contaminants, and (for the garden and forage field only) by irrigation using water from the lake or well. Contaminants leave each area by leaching, suspension, root uptake, and runoff to the lake.

- deposition to the bottom mixed sediments, and
- outflow (flushing) of the lake down-stream.

In modelling the first two of these processes, we do not actually simulate the depletion of any contaminants in the lake water by pumping or suspension. Instead, we duplicate the removed mass of contaminants and model them as if they existed simultaneously in different locations. Moreover, we include as discharge into the lake all contaminants that may arise under the terrestrial parts of the discharge zones, so that contaminants in the soil are also duplicated in the lake. These assumptions were introduced to simplify the modelling of the lake. They tend to overestimate impacts because the amount of a contaminant in the biosphere model exceeds the amount that is actually available.

Figure 5-19 identifies the two types of sediment that are modelled: compacted and mixed. Compacted sediments refer to the deep sediments directly above the overburden, and they are modelled as part of the interface between the geosphere and biosphere models (see Section 5.5).

Mixed sediments refer to the shallow sediments lying above the compacted sediments and are modelled by the lake sediment equation. The mixed sediments receive contaminants from the overlying lake water at a rate that is dependent on the concentration and chemistry of the contaminant and on the net sedimentation rate. Sedimentation occurs continuously and contributes to the bulk as well as the contaminant content of the mixed sediments.

We also consider the possibility that the fields used by the critical group might be located on fresh lake sediment. On the basis of the models and data for the reference disposal system, this possibility occurs in about 1% of the randomly sampled simulations (Davis et al. 1993). When such simulations are chosen, we assume that the concentration of contaminants in each field is the average of the estimated contaminant concentrations in the mixed and compacted sediments, weighted by the relative thicknesses of the two layers.

Important parameters used to simulate the lake and lake sediments include the rate of flushing of the lake, the rate of degassing of volatile contaminants (or gaseous evasion rates and aquatic mass loading coefficients), and the rate of removal of contaminants to the mixed sediments (Davis et al. 1993). The rate of flushing depends on the volume of the lake, the size of the watershed and the annual meteoric precipitation. The rate of removal by sedimentation depends on the sedimentation rate of particulates, the area of the lake and the extent of sorption of contaminants on particulates. The sorption coefficients for contaminants on compacted sediment are important when lake sediments are used as soil.

5.6.2.2 Well Model

The well model has already been discussed in Section 5.5, as part of the linkage between the geosphere and biosphere models. However, we mention it again because one of its parameters depends on other components of the biosphere model.

The well is an alternative to the lake as a source of water. We assume its frequency of use corresponds to current rural well usage in the Shield region of central Canada (Davis et al. 1993). Throughout each simulation of the biosphere, we assume that water used for domestic purposes, livestock and for watering the garden comes from the well or from the lake. (We also assume that the forage field may be watered but using only lake water.)

In the biosphere model, a switch parameter determines whether the critical group obtains their water from the well or from the lake. (A switch parameter is one that describes mutually exclusive options available for a simulation. It is characterized by a PDF that incorporates the relative probabilities of occurrence of each option.) When the well option is selected, the biosphere model determines the volume of water tentatively required from the well. This tentative well demand is then compared with the capacity of the well to supply water (calculated in the geosphere model). If the well cannot provide sufficient water, we decrease the well demand and assume that the difference is made up with water from the lake (Section 5.5). We use this reduced well demand when estimating concentrations of contaminants in well water.

There are several important parameters associated with the well model. One is the switch parameter that selects the source of domestic water. In this instance, the switch parameter describes one of two options: the source of domestic water is either the well or the lake. When a well is selected, another important parameter is the tentative well demand. It is determined in the biosphere model from the requirements of the critical group for water and is a function of the size of the critical group, the number of livestock, and the amount of irrigation water required to supplement meteoric precipitation.

5.6.2.3 Soil Model

The biosphere model simulates contaminant movement in the soil of four fields (Figure 5-16): a garden, a forage field on which feed and fodder for domestic and wild animals is grown, and a woodlot and peat bog that supply wood and peat for construction and heating (Sheppard 1992).

Figure 5-20 illustrates the processes simulated in the soil model. Contaminants enter field soils by three processes:

- groundwater discharge at the water table below the soil,
- air deposition of contaminants that have been released into the atmosphere from the surface of the lake, and
- irrigation using water from the lake or well (only the garden and forage field have a probability of being irrigated in the assessment of the reference disposal system, reflecting current practices).

Contaminant concentrations in the soil also increase or decrease because of radioactive decay. Contaminants may leave field soils by

- uptake in the roots of harvested plants; and
- degassing of volatile contaminants (also known as gaseous evasion), or suspension of contaminated particulates in the atmosphere.

We model the soil in each field on the assumption that it consists of four successive layers. The top two layers make up the plant rooting zone at the soil surface. The other two layers are an intermediate soil layer and a deep zone in contact with the water table. The model uses equations that summarize the results from a more detailed soil model called SCEMR1 (Sheppard 1992, Davis et al. 1993). The SCEMR1 model simulates the long-term net result of daily movement of pore water and contaminants resulting from capillary rise, root uptake, leaching and runoff, and the sorption of contaminants on soil solids. The soil model also uses the results from SCEMR1 to estimate the net requirements for irrigation water, based on soil type, field moisture capacity, evapotranspiration, runoff and meteoric precipitation.

In the soil model, we do not deplete the soil of any contaminants that may be removed by suspension (Sheppard 1992). Instead, the mass of suspended contaminants is duplicated in the soil and in the atmosphere. This assumption, introduced to simplify the modelling, leads to an overestimate of impacts that depend on contaminant concentrations in soil.

The results of these calculations include estimates of contaminant concentrations in the plant rooting zone and the net requirements for irrigation water.

Important parameters in the soil model are the soil type, soil depth, the areas of the four fields, effective meteoric precipitation, volume of irrigation water, and the extent of sorption of contaminants on the soil solids. The four types of soil are sand, loam, clay and organic, with the additional possibility that fresh lake sediments may be used instead as soil (Davis et al. 1993).

5.6.2.4 Atmosphere Model

The biosphere model calculates contaminant concentrations in the outdoor and indoor air used by the critical group and the deposition rates of contaminants onto underlying surfaces (Amiro 1992b). Figure 5-21 illustrates the atmospheric processes simulated.

We assume that the noble gases ^{39}Ar, ^{81}Kr, ^{85}Kr and ^{222}Rn discharge from the geosphere directly into the surrounding atmosphere (Davis et al. 1993). Other contaminants enter outdoor air

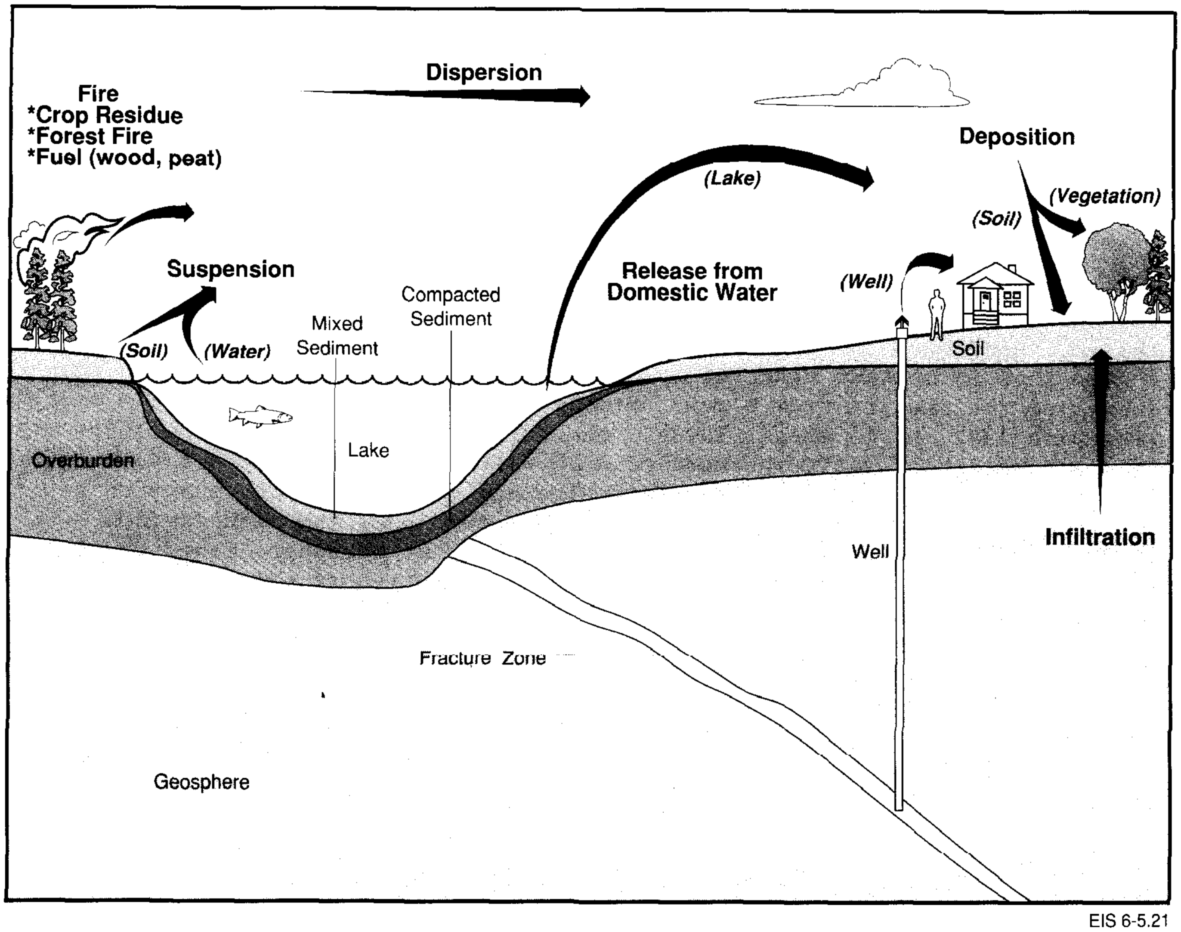

FIGURE 5-21: The Processes Modelled in the Atmosphere Model

The arrows show processes that are explicitly modelled in the atmosphere model (Davis et al. 1993). Contaminants enter outside air by degassing and suspension of particulates from the soil in the fields, from the water of the lake and from fires (including burning wood and peat for fuel). Contaminants enter dwellings with the outside air, by releases from domestic water (from the lake and the well), and by infiltration from soil around building foundations. We assume that the contaminants are well mixed by dispersion in the air.

- by degassing of volatile contaminants (also known as gaseous evasion) and suspension of contaminated particulates from soil areas and from lake water; and

- by release in smoke from burning contaminated vegetation and fuel (wood and peat).

Contaminants enter indoor air

- by infiltration of outside air;,

- in releases from domestic water, such as showers and humidifiers; and

- by infiltration from the underlying soil (for radon gas).

We assume that all contaminated particulates entering the atmosphere are eventually deposited back onto the area from which they originated (the surface of the fields or the lake). The application of this assumption means that there is a duplication in the mass of contaminants in the atmosphere and in the soil and lake.

Concentrations from particulates in the outdoor and indoor air are modelled using simple algebraic expressions (Amiro 1992b, Davis et al. 1993). The equations assume that contaminants are well mixed and their concentrations in air are proportional to their concentrations from the source. Concentrations from volatile contaminants and from contaminants released by fires are calculated in a similar manner.

Important parameters in the atmosphere model describe the rates at which contaminated particulates and volatile contaminants enter air from soils and the lake, the frequency of fires, contaminant emission rates from fires, and the dispersion of contaminants in the atmosphere (Davis et al. 1993).

5.6.2.5 Food-Chain and Dose Model for the Critical Group

The food-chain and dose model uses the concentrations of radionuclides from the lake, well, soil and atmosphere models, and the deposition rates from air and irrigation, to estimate the degree of contamination of plants and animals (Zach and Sheppard 1992). It then estimates annual dose to a member of the critical group.

We assume in the biosphere model that contaminants may reach the critical group through 23 possible exposure pathways (Table 5-2). For example, the group may receive an internal radiation dose by inhaling contaminated air or by consuming

- water from the lake or the well;

- garden plants contaminated through their roots or through their leaves;

- meat, milk and poultry products contaminated by animals' drinking water, by ingested soil or by plants derived from the forage field (the plants may be contaminated through their roots or through their leaves);

- fish from the lake; and

- contaminated soil residues on food.

The group may also receive an external dose from being near contaminated air, water, ground and building materials.

5.6.2.6 Internal Pathways

The critical group obtains all its air, water and food from the vicinity of groundwater discharges from the hypothetical vault (Davis et al. 1993).

The inhalation rate and food and water ingestion rates of individuals in the critical group are calculated from human energy requirements (Zach and Sheppard 1992). We assume that their diet consists solely of locally produced plants and berries, animal products (domestic and game meat, dairy products, poultry and eggs), fish and water. In addition, their diet includes inadvertently ingested soil. We assume that the animals supplying food to the critical group also have a diet of local produce and water, including ingested soil.

We simulate the processes leading to the accumulation of contaminants in food using algebraic equations (Zach and Sheppard 1992, Davis et al. 1993). The concentrations of contaminants in plants are calculated using concentrations in soil and air, and the following additional parameters:

- plant/soil concentration ratios (also known as soil-to-plant concentration factors and soil/plant transfer coefficients) that give contaminant concentrations in plants relative to concentrations in the soil on which they grow; and

- rates of deposition, times of above-ground exposure and interception fractions that give concentrations in plants resulting from deposition on leaves from the air and from irrigation.

The concentrations of contaminants in animals are calculated using

- the amounts of food, water and soil eaten by beef cattle, dairy cows and poultry;

- the extent of contamination of the plants (also produced locally), water and soil they eat; and

- plant-to-animal transfer coefficients to describe the portion of an ingested contaminant that is incorporated into the animal product (examples include the plant-to-milk transfer factor, the plant-to-poultry product transfer factor and the plant-to-mammalian-meat transfer factor).

The concentrations of contaminants in fish are calculated using a water-to-fish transfer factor (also known as an aquatic concentration ratio) that describes contaminant uptake from lake water by fish.

Loss and ingrowth due to radioactive decay are taken into account for the interval between the time that foodstuffs are removed from the contaminating source and the time that they are ingested.

Internal Dose Estimates

We calculate radiation doses to the critical group via internal exposure pathways from radionuclide concentrations in plants, animals, fish, water and air, using estimates of the amounts of these that would be consumed or inhaled. These calculations require dose conversion factors (DCFs) that convert the concentrations of radioactive contaminants into 50-year committed effective dose equivalents. Documentation for the dose conversion factors is provided by Zach and Sheppard (1992) and Davis et al. (1993); these factors are calculated using procedures and data from the ICRP (1977, 1979). Section E.2 in Appendix E discusses recent changes to the recommendations of the ICRP.

We take into account two special considerations in calculating the doses resulting from ^{129}I (Zach and Sheppard 1992, Davis et al. 1993): the absolute upper limit and isotopic dilution.

Nearly all of the body's iodine is concentrated in the thyroid gland, which can contain only a limited amount of iodine. Thus there is a limit to the dose that can be normally produced by ^{129}I in the body, even if all the iodine present were ^{129}I. This maximum annual dose is about 38.6 mSv/a (Zach and Sheppard 1992) and is an absolute upper limit implemented in the food-chain and dose model.

The human body requires about 200 μg of iodine per day that is either naturally present in food and water or frequently added as a dietary supplement. The biochemical processes of humans and animals do not distinguish between the isotopes of iodine, including radioactive ^{129}I and the stable isotope, ^{127}I. Consequently, the isotopes of iodine are retained in the body in the same proportion as in their sources (primarily drinking water and foods). The presence of ^{127}I reduces the amount of ^{129}I that could be retained by the body in the ratio of the concentrations of the two isotopes. This process is called isotopic dilution. We include the effects of isotopic dilution for iodine in two separate calculations, both of which yield conservative estimates of dose:

- We first use a value for ingested stable iodine (^{127}I) of 200 μg of iodine per day (Zach and Sheppard 1992, Davis et al. 1993), together with the estimated amounts of ^{129}I ingested in contaminated food and water. This calculation is called the ingested food limit for ^{129}I.

- We then repeat the calculation, but this time we assume that the critical group ingests only the iodine found in their drinking water. This water may contain ^{129}I from the disposal vault. However, it does contain concentrations of ^{127}I derived from the surrounding geosphere, and we use a PDF to describe the variability in the concentrations of ^{127}I observed in deep groundwater near the hypothetical vault in the WRA (Gascoyne and Kamineni 1992, Davis et al. 1993). This calculation is called the groundwater limit for ^{129}I. (Note that this calculation ignores sources of stable iodine other than groundwater sources; the inclusion of additional sources would further reduce actual internal doses from ^{129}I.)

We then compare the estimated annual doses that are due to ^{129}I from the ingested food limit and from the groundwater limit and choose the smaller of the two to represent the estimated annual dose from ingestion of ^{129}I. The choice may change from one simulation to the next, or even at different times for the same simulation, because of the uncertainties associated with the sampled parameters.

We have also implemented a groundwater limit for ^{14}C. The biochemical processes of humans and animals use carbon to build body tissue and do not distinguish between radioactive ^{14}C and the stable isotope, ^{12}C. Consequently, the carbon isotopes are retained in the body in the same proportion as in their sources of carbon. Thus we include a groundwater limit of dose from ^{14}C to describe the isotopic dilution of ^{14}C with ^{12}C (Zach and Sheppard 1992, Davis et al. 1993).

Important parameters in the internal exposure pathways are inhalation rates, food and water consumption rates, composition of diet, soil-to-plant and plant-to-animal transfer rates, and the factors converting ingestion rate for each radionuclide to internal dose. Other important parameters that affect the food-chain model calculations are the number of people in the critical group and the source of drinking water (Davis et al. 1993).

Finally, as discussed above, several important parameters pertain to only ^{129}I and ^{14}C. For ^{129}I, they are the maximum amount of iodine retained in the body, the amount of iodine found in the daily diet of the critical group, and the concentration of ^{127}I in groundwater. For ^{14}C, an important parameter is the concentration of stable carbon in groundwater. The concentrations of stable iodine and carbon in groundwater vary from site to site on the Canadian Shield; for consistency with the geosphere model, we use data based on observations at the WRA (Davis et al. 1993).

5.6.2.7 External Pathways

We assume that in the food-chain and dose model that the critical group may also receive an external dose from contaminants in their surroundings: the air (indoors and outdoors), water (bathing and swimming), the soil, and from building materials derived from trees or soil. Bathing and swimming involve domestic water. Wooden building materials consist of wood from the woodlot and inorganic building materials are made from soil from the forage field (which is composed of lake sediment in some instances).

External Dose Estimates

We estimate external dose to the critical group from contaminant concentrations in the surroundings such as exposure to radiation from the soil as a result of standing on the most contaminated field (Zach and Sheppard 1992).

Important parameters for external pathways calculations are the dose conversion factors that convert concentrations of external radioactive contaminants to effective dose equivalents for each radioisotope in soil, air and water, and estimates of the duration of exposure to each external source (Davis et al. 1993).

5.6.2.8 Dose Model for Other Organisms

We also estimate the radiation dose to nonhuman biota from ingestion and external exposure pathways in the biosphere model. The primary reference for the biosphere model (Davis et al. 1993) outlines how conservative estimates of radiation dose are calculated for specific target organisms. These calculations require a large amount of data, some of which are not readily available. Thus we have relied on a generic approach for the post-closure assessment; this approach is well supported by data and addresses environmental protection in an integrated and holistic manner.

The dose model for nonhuman biota considers four generic target organisms (Davis et al. 1993):

- A plant with contaminant uptake characteristics similar to a broad range of terrestrial vascular plants, including many grasses, herbs and trees. The soil-to-plant and air-to-plant pathways involve contaminant uptake from soil, and deposition onto leaves from the atmosphere and irrigation water. For external exposures, the plant is immersed in air, soil and water. This reflects a broad range of terrestrial and aquatic plants and includes exposure of the roots, shoots, leaves and reproductive parts.

- A mammal most similar to a herbivore in its eating habits. Typical species include caribou, moose, beaver and meadow vole. The mammal accumulates nuclides from ingestion of water, vegetation and soil. Higher levels of consumers, such as predators, are not modeled explicitly; they would be included, to a certain extent, in the broad distribution of transfer factors. External exposure of mammals includes immersion in water, air, soil and vegetation, and thus encompasses terrestrial, semiaquatic and soil-burrowing mammals.

- A bird most similar to a terrestrial species that eats seeds and fruit. Typical species include ruffed grouse, song sparrow and evening grosbeak. The ingestion and external exposure pathways considered are the same as for the mammal.

- Fish representing a wide range of free-swimming and bottom-feeding species, including lake trout, northern pike, lake whitefish and white sucker. The fish inhabiting the discharge lake might become contaminated through the ingestion of food and sediment and through osmotic exchange of fluids. The fish may also receive an external radiation dose from water and from lake-bottom sediments.

Each of these biota are located in the immediate discharge zones of the reference disposal vault, and in this sense they are "critical" biota, similar to the critical group.

Calculated concentrations of radionuclides in surface water, soil and air are used to estimate radionuclide concentrations in tissues of the target organisms through use of the food-chain transfer coefficients. The concentrations in the tissues are then related in a conservative manner to radiation dose from exposure to internal sources using DCFs (Davis et al. 1993). The concentrations in surface water, soil and air are also used to calculate radiation dose from exposure of the organism to external radiation sources. Inhalation exposures have not been evaluated but are expected to be of much less importance (Davis et al. 1993).

The dose equations are similar to those for the human dose pathways, with two slight differences:

- No nuclide losses resulting from decay during a holdup time are included because the organisms receive a dose as soon as they take in the nuclide or are exposed to it in their habitat.

- Radiation doses to the target organisms are calculated in units of gray. The basic unit of absorbed dose of ionizing radiation is the gray (ICRP 1977, Davis et al. 1993). For humans, we report annual dose (more precisely the annual effective dose equivalent) in Sv/a, which takes into account the biological consequences on humans of different types of radiation. The sievert is the product of the dose in grays and a dimensionless radiation quality factor that describes the effectiveness of different types of radiation in producing biological effects on humans. The quality factor has a value of unity for ^{129}I, ^{14}C and ^{99}Tc for humans (Davis et al. 1993), but equivalent data are not well known for nonhuman biota.

In applying the equations, we consider only three contaminants: ^{129}I, ^{14}C and ^{99}Tc, which are the nuclides of most concern for the reference disposal system. In fact, the results of the assessment discussed in Sections 6.2 to 6.5 show that only ^{129}I and ^{14}C have significant concentrations in any parts of the biosphere (^{99}Tc produces small concentrations in some sensitivity analyses).

Although a rigorous methodology to relate radiation dose to risk for nonhuman biota does not exist, we can compare estimated radiation doses for the generic organisms with doses where effects have or have not been observed in the laboratory or field.

5.7 DATA USED BY THE MODELS

For the models discussed in Sections 5.1 to 5.6, we identified many of the parameters that are used in the postclosure assessment to provide estimates of impacts from the reference disposal system. In this section, we discuss the data for the input parameters. An input parameter is one that requires supplied data; other parameters (or variables), such as contaminant concentrations and estimates of annual dose, are calculated from these input parameters.

The geochemical, geological and hydrological features of the reference disposal system are based on extensive research studies at the WRA (Davison et al. 1994b). This specific site was selected to ensure that the geological data used in the assessment are realistic and self-consistent. By self-consistent, we mean that the parameter values in the system model are compatible and not contradictory. For example, the discharge locations are consistent with the detailed modelling of the WRA (Davison et al. 1994b), and these discharge locations are used by both the geosphere and biosphere models. Similarly, groundwater velocities and rock properties used by the vault model are consistent with those used in the geosphere model and are based on results of the research studies from the WRA.

The biosphere model is largely generic; thus it involves but does not specifically model the WRA (except for features such as discharge locations and concentrations of stable iodine and carbon in groundwater). Data for the biosphere model are derived from the literature and from a variety of field and laboratory studies, selected to represent the Shield environment of central Canada.

To select appropriate data for the parameters of the system model, we must deal with several issues:

- The complete set of site characteristics and facility design cannot be completely specified. Data for some parameters may not be known, and data for others may be uncertain or variable (and vary over a wide range).

- Field and laboratory data always have some degree of error and uncertainty that can, in some cases, have significant implications on estimated impacts.

- Data obtained in the laboratory must be extrapolated if the conditions in the laboratory do not match the chemical and physical conditions covered in the assessment models. Extrapolation may also be required so that data obtained from short-duration experiments can be applied over the long time-scale of the assessment.

We take these features of the data into account by using a probabilistic approach in preparing quantitative estimates of effects for the postclosure assessment (Chapter 2 and Section A.3 of Appendix A). The probabilistic approach implies that we specify a distribution of allowed values for each sampled parameter. The distributions are specified using PDFs:

> A PDF is a function defined over the range of values for a parameter. It is equal to zero for any parameter value that researchers believe is impossible; these values will never be selected for a simulation. The PDF function is greater than zero for any parameter value that researchers believe is possible.

> These values may be sampled for a simulation. If one parameter value is thought to be more likely than another, then its weighting in the PDF function will be larger, and the value will tend to be sampled more frequently.

That is, PDFs are chosen to include the credible range of values for the sampled parameters and to provide the likelihood of occurrence of specific values of the parameter within this range.

Some properties can vary from place to place, like rock permeability, or from time to time, like annual rainfall. The parameter value corresponding to such a property is chosen as a single time-independent value for a simulation. The models in SYVAC3-CC3 do not include any parameters that are both sampled and time dependent. If the time dependence of a quantity is deemed important and can be quantified, it is treated as a calculated variable and is a function of other parameters that are sampled and constant in time.

To some degree, a spatially varying property may be described by a spatial representation in the model using several related parameters. Examples in the system model for the reference disposal system are as follows.

- Each of the 12 sectors in the vault will experience a different temperature rise in the future, depending on the amount of heat-producing waste present and the location of the sector relative to other sectors and to the rock of the geosphere. This spatial variability in temperature rises is accounted for in simulating the rates of corrosion of the containers (Johnson et al. 1994b), and thus the different sectors have different rates of container failure.

- The rock between the vault and the biosphere is described using 46 segments (Section 5.4). All segments are characterized using the same types of parameters, such as permeability and the types and amounts of minerals present. However, the PDFs for the parameters in one segment differ from those of another segment, explicitly representing much of the spatial variability of the rock in the geosphere.

Some parameters represent an effective or lumped quantity that takes into account spatial or temporal variability. Their PDFs include this variability and all other sources of uncertainty. In general, for all parameters, the distribution of values defined by a PDF represents our lack of knowledge. If the PDF for an effective quantity takes into account spatial or temporal variability, then its PDF includes our uncertainty about how well values for the effective quantity would account for this variability.

We have also implemented correlations between parameters. That is, the values for some parameters are not mutually independent, but exhibit some underlying relationship. In general, we use correlation coefficients for a small number of parameters, such as the amounts of food, soil and water consumed by members of the critical group, and the frequency of irrigation of different types of soil (Davis et al. 1993).

Where possible, we describe correlations in the system model in a different way, by calculating values for correlated parameters from a more fundamental set of sampled parameters that are taken to be independent. Three examples where this approach is used in the reference disposal system are simulating precipitation in the buffer, anionic transport in the buffer and sorption on rock in the geosphere.

- The tendency of nuclides to precipitate in the buffer depends on the chemical regime, which could affect different nuclides in a similar way. For example, we expect to find that the precipitation of uranium and technetium is affected by the electrochemical potential in the buffer. In SYVAC3-CC3, we correlate solubility limits for uranium and technetium, and for plutonium, neptunium and thorium, by calculating them as a function of a basic set of sampled parameters that include electrochemical potential and other fundamental sampled parameters (Johnson et al. 1994b).

- The movement of different anionic species in the buffer is expected to be similar. For SYVAC3-CC3, researchers have correlated the buffer diffusion coefficient and the buffer capacity factor for all contaminants in the vault that form anionic species in groundwater. These parameters are correlated to an independent sampled parameter called the buffer anion correlation parameter (Johnson et al. 1994b).

- Elements with similar chemical properties have similar trends when sorbing onto the minerals in the rock of the geosphere. There is also some correlation between the extent of sorption in parts of the geosphere that are chemically similar. Sorption in the geosphere is determined, for each chemical element, as a function of more basic parameters, such as the salinity of the groundwater and the types and amounts of minerals present in a segment of rock (Davison et al. 1994b). Correlations in sorption within one segment are accounted for by the presence of different minerals within the segment (the amount of each mineral is a sampled quantity). Thus all elements that are strongly sorbed by hematite have strong sorption in a segment containing the mineral hematite. Correlations in sorption within different segments are also accounted for because of the presence of the same minerals, possibly in different amounts. For example, an element strongly sorbed by hematite is strongly sorbed in all segments containing hematite.

The selected PDF may represent a combination of field and laboratory measurements, historical data, theoretical principles and the collective opinion of experts. To ensure consistency in the data set as a whole, all data contributors were asked to apply a common set of guidelines when they defined their PDFs. The guidelines (Stephens et al. 1989, 1993) recognize the key role played by the judgment of experts in defining appropriate PDFs. It is not feasible to give detailed prescriptions or directives to be applied in defining data distributions. Instead, the guidelines consist of background information about the objectives of the postclosure assessment, a description of the reference disposal system, the assumptions made and the conditions prevailing for the assessment of the system. The guidelines also

- describe the mathematical requirements to define these PDFs, and

- provide instructions for including correlations among the values of two or more parameters.

In addition, we follow the principle that, if there is insufficient information to specify unambiguously a PDF, then the selected PDF and its attributes should bias values that would lead to overestimates of impact.

The specification of PDFs used with the reference disposal system is controlled by experts in the areas of science and engineering appropriate to each of the parameters. The PDFs chosen for all parameters are fully documented in the primary references on the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al 1993). These references also give the justification for each selection.

A final consideration affecting the postclosure assessment is the great quantity of the data that is required. The system model uses more than 7000 parameters, all requiring corresponding data. We use an automated database system (Section B.5 in Appendix B) to manage this data and to provide assurance that the data are correctly passed from the data contributor to the computer codes used in the assessment.

The database system comprises a collection of standard data-submission forms, one for each parameter or class of related parameters. For each parameter, a specific expert was assigned the responsibility for reviewing and selecting the appropriate data. Further data checks were performed by

- the Chairpersons of the Model Working Groups that developed the vault, geosphere and biosphere models;

- the personnel who were directly involved with developing the computer code for the postclosure assessment; and

- the database administrator.

These checks ensured that the data supplied by the experts were correctly installed in the database.

Copies of the forms are also stored on a computer database. The computer database can be changed only by the database administrator. An automated procedure has been established to interrogate the computer database and to extract the data needed to perform any of the calculations required for the postclosure assessment.

More details on the database system are provided in Appendix B.

5.8 PERIOD OF APPLICABILITY OF THE SYSTEM MODEL

5.8.1 Introduction

We have developed the system model to describe the release and transport of contaminants from the reference disposal system and to estimate impacts associated with the SYVAC scenarios. Our application of SYVAC3-CC3, documented in Chapter 6, yields quantitative results for times up to 10^4 a from the closure of the disposal facility. We also present results that are extrapolated to 10^5 a and report the maxima in estimated impacts for times up to 10^5 a.

Although the system model is designed to be applicable to 10^4 a, it may also be acceptable for longer times. We summarize in this section how the three models making up the system model would be affected for times beyond 10^4 a. More detailed discussions are provided in the primary references on the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993).

5.8.2 Period of Applicability of the Vault Model

The vault model is considered appropriate for estimating probable releases from the vault for the time frame up to approximately 10^5 a after closure (Johnson et al. 1994b). The following notes discuss the time frame for which some components of the vault model are expected to produce acceptable estimates (Johnson et al. 1994b):

- *Container*: Studies of the behaviour of Grade-2 titanium containers suggest that the major modes of failure would be due to initial defects, crevice corrosion and delayed hydride cracking (Johnson et al. 1994b). These modes of failure, together with several conservative assumptions, lead to the modelling result that all containers would fail within 10^4 a (although Johnson et al. (1994b) anticipate that actual failure times would be much longer than 10^4 a).

- *Used fuel*: The dissolution of used fuel is enhanced by the presence of alpha radiolysis, the chemical decomposition of molecules resulting from the release of alpha particles (Johnson et al. 1994b). Alpha radiolysis could produce oxidizing electrochemical potentials at the surface of the used fuel. After about 10^5 a, alpha activity will have decreased to a level comparable to that of a rich uranium ore deposit (Johnson et al. 1994b).

  In the postclosure assessment, the electrochemical potential in the vault represents the relatively oxidizing conditions that are possible at short time frames and that promote the dissolution of used fuel. At longer times, this electrochemical potential would be much less oxidizing, and the vault model would greatly overestimate the dissolution of used fuel and the associated congruent release of contaminants (Johnson et al. 1994b). Thus the vault model should not be used to estimate contaminant releases from the used-fuel matrix beyond about 10^5 a.

- *Transport in the vault*: The parameters describing contaminant transport in the buffer and backfill material reflect conditions likely to persist over a period of 10^5 a. Over much longer periods of time, the clay material (bentonite) in the buffer could slowly change to an illite clay; however, it is expected that these changes would not significantly affect transport properties (Johnson et al. 1994b).

  Estimates of transport in the vault may also be influenced through the formation of a hydrogen gas phase. Johnson et al. (1994b) estimate that this might occur some time after about 2×10^4 a, but the amount of gas would occupy only about 1% of the total pore space in the buffer and backfill, and thus should have no important effects on contaminant transport. Over longer periods of time, a slowly accumulating gas phase could have complex effects; for example, it may inhibit contaminant transport by limiting the access of water to the containers (Johnson et al. 1994b).

  Finally, the transport of contaminants out of the vault depends on the groundwater velocity in the surrounding rock, which could change with the onset of glaciation (Johnson et al. 1994b).

  The cumulative uncertainty in the effects of these processes suggests that the vault model should not be used to estimate contaminant transport in the vault for times beyond 10^5 a.

5.8.3 Period of Applicability of the Geosphere Model

The geosphere model is considered to be applicable until the onset of the next glaciation (Davison et al. 1994b). Until that time, the factors affecting the flow of groundwater and the transport of vault contaminants through the geosphere surrounding the disposal vault are expected to remain relatively constant. These factors include the hydraulic pressure field, the permeability of the rock mass and the major fracture zones within it, the chemistry of the groundwater and the chemistry of the rock and the minerals in the fractures in the rock.

Although the effects of glaciation are unlikely to disturb the physical characteristics of the rock at or below the 500- to 1000-m depth of a vault, they could affect the hydraulic pressure field or permeability of the fractures zones in the rock enough to change the groundwater flow pattern (Davison et al. 1994b, Heinrich 1984a).

Glaciation could alter both near-surface and deep groundwater flow patterns. This would render incorrect our current representation of the transport pathways through the geosphere from the vault to the biosphere. Thus the applicability of the geosphere model is considered limited to the period until the onset of the next glaciation.

5.8.4 Period of Applicability of the Biosphere Model

The major physical factor limiting the period of applicability of the biosphere model is the change in climate induced by the onset of the next glaciation or any other event that produces a significant long-term change in the present climate. The biosphere model and parameter values have been developed to simulate current interglacial conditions, which correspond to the warm periods between glaciations (Davis et al. 1993). The expected reduction in temperature and the resulting ice cover over the Shield region would render inappropriate the biosphere model used in the postclosure assessment. However, our analysis shows that it is unlikely that glaciation would lead to substantially increased impacts to humans or other biota (Davis et al. 1993).

In a general way, the biosphere model would be applicable for each of the warm periods between glaciations in the future, but the effects of the glaciations on the linkages with the geosphere (such as contaminant discharge locations) are not known. Thus the applicability of the biosphere model is limited to the present warm period. However, if it is assumed that the geosphere is largely unaffected by glaciation, then we can use the biosphere model to estimate impacts for the mild and cold interstadial periods that differ only slightly from those calculated for the current interglacial period (Davis et al. 1993).

Socio-technical factors could also affect significantly the applicability of the model, the most unpredictable being technical, social and environmental factors linking the contaminants entering the biosphere to an impact on humans and their environment. Recent cultural and technological changes have been so rapid and so profound that the possible effects on model applicability are extremely difficult to assess. Estimates of far-future living and environmental conditions are largely speculative. Thus our calculations should be viewed as an illustration of what the impacts would be if the releases occurred today, rather than as a prediction of the actual impacts in the future (in line with international opinion (NEA/IAEA/CEC 1991)). The results should be considered as indicators of safety that can be compared with safety standards. The biosphere model includes a number of conservative assumptions to cover a wide range of environmental and climate conditions and to ensure that potential impacts are not underestimated.

The expected time limit to the applicability of the biosphere model is, therefore, the onset of the next glaciation.

5.9 CONTAMINANTS OF CONCERN FOR THE POSTCLOSURE ASSESSMENT

In this section, we discuss the results of a screening study (Goodwin and Mehta 1994) used to identify the contaminants of concern for the postclosure assessment of the reference disposal system. The study corresponds to a preliminary application of the fourth step of estimating impacts in our assessment approach (see Figure 2-1). It is considered to be preliminary because the study did not use the relatively detailed models described in the previous section, but rather it used simple models (and associated data) that are extremely conservative. That is, the screening study used models and data that lead to overestimates of the potential impacts (and that are more conservative than the models and data described in Sections 5.1 to 5.6). The study was carried out so that the development of more detailed models would be focussed on the most important contaminants, some of which require special modelling considerations.

In the following discussion, we first discuss the source of the contaminants, review the screening calculations, and then list the contaminants of concern for the postclosure assessment. These contaminants are examined in more detail in Sections 6.2 to 6.6.

5.9.1 Sources of Contaminants

The postclosure assessment is focussed on contaminants originating in used-fuel bundles from CANDU nuclear generating stations. Thus we have examined the contaminant inventory in irradiated uranium dioxide (UO_2) fuel and the Zircaloy sheaths used to contain the fuel.

For modelling purposes, we assume that all fuel bundles would have the following characteristics (Johnson et al. 1994b):

- they contain the same type and amount of contaminants;

- they are of the type produced by the Bruce Nuclear Generating Station;

- they have each produced thermal energy amounting to 685 GJ/kg of initial uranium; and

- they have been stored out of the reactor for at least 10 a, so that their level of heat and radiation emission is much lower than when they were in the reactor. Thus using a value of 10 a will lead to an overestimate of the temperature rise in the vault, and subsequently to an overestimate of the rates of corrosion and failure of the containers. (It is anticipated that most, if not all, of the bundles will have been in storage much longer than a decade.)

An actual disposal system would contain fuel bundles with somewhat different characteristics, partly because the bundles may come from other CANDU reactors. We expect these differences will not have a large effect on the results of the postclosure assessment. In addition, the inventories of contaminants considered in the postclosure assessment are described using PDFs (Johnson et al. 1994b), which should encompass most of these differences.

Potential contaminants in these reference fuel bundles include the original uranium dioxide and constituents of Zircaloy, plus

- Fission products originating from the consumption of the UO_2 fuel and neutron activation products of impurities (that is, elements other than uranium and oxygen) in the UO_2 fuel;

- Neutron activation products of nuclides (including impurities) in the Zircaloy sheaths; and

- Members of the four actinide decay chains, which originate from the neutron activation of the isotopes of uranium.

5.9.2 Review of the Screening Calculations

After use in a nuclear reactor, UO_2 fuel and Zircaloy sheaths contain hundreds of potential contaminants. However, not all contaminants are of concern. Many are not radioactive, and their chemical toxicity may be negligible as well. Other contaminants are radioactive, but their radiotoxicity hazard is negligible because they are present in very small amounts or because they decay away in a short period of time.

To identify the contaminants of concern for the postclosure assessment, Goodwin and Mehta (1994) calculated overestimates of potential impacts from more than 151 radionuclides and more than 80 chemical elements associated with irradiated UO_2 fuel and Zircaloy sheaths. Their calculations use a number of extremely conservative assumptions; for example, they assumed the entire inventories of all contaminants are released instantly from the used-fuel and Zircaloy matrices at the time of closure; there are only 25 m of sparsely fractured rock between the vault and a well used by the critical group; all contaminants leaving the vault reach the well; the well supplies just enough water for one individual, and this water is the sole source of drinking water for that individual; and all the contaminants reaching the well also accumulate in just enough soil needed to supply food to one individual who consumes all the accumulated contaminants within 50 a. Many of these assumptions were made to simplify the modelling process. Their calculations also use parameter values chosen to overestimate impacts.

These very conservative calculations are used to screen the contaminants and identify those requiring further evaluation in this report.

- The study provided (over-)estimates of the concentrations of contaminants in water and soil from chemically toxic contaminants. We decided that a chemical element requires further study in the postclosure assessment if its estimated concentrations in water or soil exceed existing guidelines or regulations. Some other considerations, such as the natural abundance of elements in a granite rock, are also used to obtain a short list of chemical elements of most concern for their potential chemical toxicity impacts (Goodwin and Mehta 1994).

- The screening study also provided (over-)estimates of annual doses to humans from ingestion of contaminants in water and soil. We decided that a radioactive contaminant requires further study in the postclosure assessment if its upper bound is greater than 5×10^{-8} Sv/a at any time up to 10^5 a (this annual dose is 1000 times smaller than the annual dose to 10^4 a associated with the AECB radiological risk criterion).

(The screening study considered inventory data reported by Tait et al. (1989) and concluded that ^{36}Cl does not require further consideration in the postclosure assessment (Goodwin and Mehta 1994). This conclusion is now being re-examined because recent information indicates that there may be additional ^{36}Cl in the used-fuel bundles, associated with the neutron activation of ^{35}Cl impurities in the UO_2 fuel pellets, in the Zircaloy sheaths and in related materials. The potential impacts of ^{36}Cl are now being evaluated, and will be documented in another report. However, ^{36}Cl is expected to behave much like ^{129}I in the disposal system, and bounding calculations indicate that radiation doses attributed to ^{36}Cl would be comparable to radiation doses resulting from ^{129}I. Chemical toxicity impacts from Cl are unlikely.)

5.9.3 Chemically Toxic Contaminants of Concern

Table 5-3 lists the nine chemically toxic contaminants of concern for the postclosure assessment. Goodwin and Mehta (1994) identified eight elements that are of most concern: antimony, bromine, cadmium, chromium, cesium, molybdenum, selenium and technetium. (Technetium is found in both the used-fuel and Zircaloy matrices. We consider only the former, because the

TABLE 5-3

CHEMICALLY TOXIC ELEMENTS INCLUDED IN THE POSTCLOSURE ASSESSMENT OF THE REFERENCE DISPOSAL SYSTEM

Element*	Source**	Inventory*** mol/kg U
Br	F	6.56×10^{-5}
Cd	F	1.18×10^{-4}
Cr	Z	2.16×10^{-3}
Cs	F	4.20×10^{-3}
Mo	F	8.23×10^{-3}
Sb	F	1.99×10^{-5}
Se	F	1.61×10^{-4}
Sm	F	1.46×10^{-3}
Tc	F	2.07×10^{-3}

* The identification of these elements is based on a screening study by Goodwin and Mehta (1994).

** The abbreviations for the sources of the elements are:
F - fission products of UO_2 fuel or neutron activation products of fuel impurities, and
Z - neutron activation product of Zircaloy materials.

*** The last column lists the assumed element inventories, in mol/kg of initial uranium. The values listed are median values from the PDFs used in the postclosure assessment of the reference disposal system (Johnson et al. 1994b).

inventory of technetium in Zircaloy is about 5 orders of magnitude smaller than its inventory in used fuel.) We have added samarium to the list because it was identified as being potentially important in an earlier study of chemically toxic elements (Goodwin et al. 1987b).

5.9.4 Radionuclides of Concern

Table 5-4 lists the 68 radioactive isotopes, or radionuclides, that are examined explicitly in this assessment. Sixty were identified by the screening study described above (Goodwin and Mehta 1994). An additional 8 radionuclides (^{241}Am, ^{113m}Cd, ^{182}Hf, ^{94}Nb, ^{125}Sb, ^{182}Ta, ^{125m}Te and ^{93}Zr) are included in our assessment because they had been tentatively recommended in an earlier study.

Thirty-three radionuclides are associated with the actinide decay chains. Thirteen radionuclides appear twice in the table (for a total of 81 entries) because they are found in both the UO_2 fuel and Zircaloy sheaths and have different rates of release from the two waste matrices (Section 5.2).

Most of the 68 radionuclides decay directly to stable isotopes (or decay through very short-lived progeny to stable isotopes), but some are members of decay chains. Many decay chains are simple and can be represented by pairs of radionuclides: precursors and progeny. These progeny and precursors pairs are

- ^{93m}Nb (progeny) from the radioactive decay of ^{93}Mo (precursor) and from ^{93}Zr (another precursor),
- ^{32}P from ^{32}Si,
- ^{126}Sb from ^{126}Sn,
- ^{182}Ta from ^{182}Hf,
- ^{125m}Te (from ^{125}Sb), and
- ^{90}Y from ^{90}Sr.

Goodwin and Mehta (1994) show that all these progeny radionuclides can be assumed to be in secular equilibrium with their precursors in some parts of the system model. The meaning of secular equilibrium is described below.

The four actinide decay chains are more complex because each typically includes more than 10 radionuclides. However, they can be simplified for the postclosure assessment of the reference disposal system to the chains shown in Figure 5-22, when these simplifications are accompanied by adjustments to some radionuclide inventories and dose conversion factors (Goodwin and Mehta 1994). The required adjustments are used in the postclosure assessment. The corresponding data are described in the primary references for the vault model (Johnson et al. 1994b) and for the biosphere model (Davis et al. 1993). These adjustments mean that more than 35 radionuclides, other than those listed in Table 5-4, are implicitly included in the postclosure assessment.

TABLE 5-4

RADIONUCLIDES INCLUDED IN THE POSTCLOSURE ASSESSMENT OF THE REFERENCE DISPOSAL SYSTEM

Radionuclide[1]	Source[2]	Half-Life[3] (a)	Inventory[4] (mol/kg U)
^{225}Ac	4n+1	2.74×10^{-2}	1.20×10^{-19}
^{227}Ac	4n+3	2.18×10^{1}	1.71×10^{-14}
^{241}Am	4n+1	4.32×10^{2}	3.62×10^{-04}
^{39}Ar	F	2.69×10^{2}	2.03×10^{-10}
^{10}Be	F	1.6×10^{6}	8.54×10^{-10}
^{10}Be	Z	1.6×10^{6}	1.67×10^{-10}
^{208}Bi	Z	3.68×10^{5}	9.66×10^{-14}
^{210}Bi	4n+2	1.37×10^{-2}	2.28×10^{-19}
^{210m}Bi	Z	3.0×10^{6}	1.44×10^{-12}
^{14}C	F	5.73×10^{3}	1.84×10^{-5}
^{14}C	Z	5.73×10^{3}	3.27×10^{-6}
^{41}Ca	F	1.4×10^{5}	1.31×10^{-6}
^{113m}Cd	F	1.36×10^{1}	1.74×10^{-7}
^{135}Cs	F	2.3×10^{6}	1.76×10^{-4}
^{3}H	F	1.24×10^{1}	2.76×10^{-6}
^{3}H	Z	1.24×10^{1}	3.20×10^{-11}
^{182}Hf	Z	9.0×10^{6}	2.20×10^{-8}
^{129}I	F	1.57×10^{7}	3.47×10^{-4}
^{40}K	F	1.28×10^{9}	2.21×10^{-7}
^{81}Kr	F	2.1×10^{5}	6.73×10^{-11}
^{85}Kr	F	1.07×10^{1}	3.69×10^{-5}
^{93}Mo	F	3.5×10^{3}	1.62×10^{-9}
^{93}Mo	Z	3.5×10^{3}	2.51×10^{-9}
^{93m}Nb	F	1.36×10^{1}	0.0
^{93m}Nb	Z	1.36×10^{1}	0.0

continued...

TABLE 5-4 (continued)

Radionuclide[1]	Source[2]	Half-Life[3] (a)	Inventory[4] (mol/kg U)
^{94}Nb	Z	2.03×10^{4}	6.40×10^{-7}
^{59}Ni	F	7.5×10^{4}	3.55×10^{-6}
^{59}Ni	Z	7.5×10^{4}	1.02×10^{-6}
^{63}Ni	F	9.6×10^{1}	5.98×10^{-7}
^{63}Ni	Z	9.6×10^{1}	1.73×10^{-7}
^{237}Np	4n+1	2.14×10^{6}	1.12×10^{-3}
^{32}P	F	3.91×10^{-2}	0.0
^{32}P	Z	3.91×10^{-2}	0.0
^{231}Pa	4n+3	3.286×10^{4}	1.33×10^{-10}
^{233}Pa	4n+1	7.39×10^{-2}	5.65×10^{-12}
^{205}Pb	Z	1.43×10^{7}	2.29×10^{-9}
^{210}Pb	4n+2	2.23×10^{1}	3.71×10^{-16}
^{107}Pd	F	6.5×10^{6}	5.08×10^{-4}
^{210}Po	4n+2	3.79×10^{-1}	6.31×10^{-18}
^{238}Pu	4n+2	8.77×10^{1}	2.02×10^{-5}
^{239}Pu	4n+3	2.41×10^{4}	1.15×10^{-2}
^{240}Pu	4n	6.54×10^{3}	4.29×10^{-3}
^{241}Pu	4n+1	1.44×10^{1}	5.94×10^{-4}
^{242}Pu	4n+2	3.76×10^{5}	2.50×10^{-4}
^{223}Ra	4n+3	3.13×10^{-2}	2.45×10^{-17}
^{224}Ra	4n	1.0×10^{-2}	2.05×10^{-14}
^{225}Ra	4n+1	4.05×10^{-2}	1.78×10^{-19}
^{226}Ra	4n+2	1.6×10^{3}	2.63×10^{-13}
^{228}Ra	4n	5.75×10^{0}	1.75×10^{-19}
^{87}Rb	F	4.7×10^{10}	6.31×10^{-4}

continued...

TABLE 5-4 (continued)

Radionuclide[1]	Source[2]	Half-Life[3] (a)	Inventory[4] (mol/kg U)
^{187}Re	Z	5.0×10^{10}	2.69×10^{-6}
^{222}Rn	4n+2	1.05×10^{-2}	1.72×10^{-18}
^{125}Sb	F	2.77×10^{0}	1.87×10^{-6}
^{125}Sb	Z	2.77×10^{0}	1.12×10^{-7}
^{126}Sb	F	3.40×10^{-2}	0.0
^{79}Se	F	6.5×10^{4}	1.64×10^{-5}
^{32}Si	F	4.50×10^{2}	1.52×10^{-14}
^{32}Si	Z	4.50×10^{2}	3.88×10^{-15}
^{126}Sn	F	1.0×10^{5}	3.92×10^{-5}
^{90}Sr	F	2.91×10^{1}	1.13×10^{-3}
^{182}Ta	Z	3.15×10^{-1}	0.0
^{99}Tc	F	2.13×10^{5}	2.07×10^{-3}
^{99}Tc	Z	2.13×10^{5}	2.63×10^{-8}
^{125m}Te	F	1.59×10^{-1}	0.0
^{125m}Te	Z	1.59×10^{-1}	0.0
^{227}Th	4n+3	5.12×10^{-2}	3.96×10^{-17}
^{228}Th	4n	1.91×10^{0}	3.91×10^{-12}
^{229}Th	4n+1	7.34×10^{3}	3.22×10^{-14}
^{230}Th	4n+2	7.7×10^{4}	5.52×10^{-9}
^{231}Th	4n+3	2.91×10^{-3}	3.55×10^{-14}
^{232}Th	4n	1.41×10^{10}	9.99×10^{-10}
^{234}Th	4n+2	6.60×10^{-2}	6.11×10^{-11}
^{232}U	4n	7.2×10^{1}	1.80×10^{-10}
^{233}U	4n+1	1.59×10^{5}	9.26×10^{-10}
^{234}U	4n+2	2.45×10^{5}	2.04×10^{-4}

continued...

TABLE 5-4 (concluded)

Radionuclide[1]	Source[2]	Half-Life[3] (a)	Inventory[4] (mol/kg U)
^{235}U	4n+3	7.04×10^{8}	8.58×10^{-3}
^{236}U	4n	2.34×10^{7}	3.25×10^{-3}
^{238}U	4n+2	4.47×10^{9}	4.14×10^{0}
^{90}Y	F	7.30×10^{-3}	2.84×10^{-7}
^{93}Zr	F	1.53×10^{6}	1.81×10^{-3}
^{93}Zr	Z	1.53×10^{6}	1.95×10^{-4}

1 Radionuclides are abbreviated using their atomic mass number and element symbol; for example ^{238}U identifies the isotope of uranium containing a total of 238 neutrons and protons in its nucleus. Some isotopes may have more than one long-lived energy state, and we add the character "m" (for metastable) to the atomic mass number for the isotope with the higher energy. For example, ^{93m}Nb has a higher energy than ^{93}Nb. In this case, ^{93m}Nb is radioactive and decays to ^{93}Nb which is stable.

There are 68 unique radionuclides from 40 elements. Thirteen of the radionuclides appear twice because they occur in both the UO_2 fuel and in the Zircaloy sheaths.

2 The abbreviations for the sources of the radionuclides are
- F - fission products of UO_2 fuel or neutron activation products of fuel impurities (28 radionuclides);
- Z - neutron activation products of Zircaloy materials (20 radionuclides); and
- 4n, 4n+1, 4n+2, 4n+3 - formulae that identify the four actinide decay chains (with 7, 8, 11 and 7 radionuclides respectively), which are simplified as shown in Figure 5-22. These formulae give the mass numbers of members in a chain, where n is an integer. For example, ^{238}U, ^{234}U and ^{230}Th are members of the 4n+2 chain; ^{239}Pu and ^{235}U belong to the 4n+3 decay chain.

3 Half-life values are taken from ICRP-38 (ICRP 1983). Several different values are reported for the half-life of ^{32}Si; for example, Walker et al. (1989) give a value of 100 a.

4 The radionuclide inventories, in moles per kilogram of initial uranium, are median values from the PDFs used in the postclosure assessment of the reference disposal system (Johnson et al. 1994b). Inventories for some short-lived radionuclides (such as ^{93m}Nb) are reported as zero, indicating that they are of concern only because of ingrowth from a precursor, and not from their initial inventory. Inventories of some radionuclides are larger than than those reported by Tait et al. (1989) because they include contributions from precursors (Johnson et al. 1994b).

Figure 5-22 also indicates that some radionuclides in the actinide chains can be modelled using the secular-equilibrium approximation. Secular equilibrium is invoked to simplify the modelling of some radionuclides. It is employed in the different components of the system model for the reference disposal system when two conditions are met: the half-life of a progeny must be much less than the half-life of its precursor and both the precursor and progeny must reside within some medium for times longer than about 4 times the half-life of the progeny. When these conditions are met, their activities are approximately equal, so that the mass of the progeny in that medium is approximately equal to the mass of its precursor times the ratio of the progeny half-life to the precursor half-life (Goodwin and Mehta 1994).

We use the secular-equilibrium approximation in the vault and geosphere models, including the overburden and compacted lake sediment. It means that we do not explicitly simulate the movement of nuclides such as ^{90}Y in these parts of the system model; instead, we can estimate the mass of ^{90}Y that enters the biosphere model from the simulation results for ^{90}Sr.

6. QUANTITATIVE ASSESSMENT OF THE REFERENCE DISPOSAL SYSTEM

6.1 OVERVIEW OF THE ANALYSIS

This chapter presents the quantitative analysis of results for the post-closure assessment of the reference disposal system, a hypothetical implementation of the concept for disposal of Canada's nuclear fuel waste. The analysis involves two steps from the assessment procedure shown in Figure 2-1: estimating impacts and analyzing sensitivity.

Much of the quantitative analysis is for the SYVAC scenarios and uses the models and data described in Chapter 5 and implemented in the SYVAC3-CC3 computer code. The analysis for the SYVAC scenarios is divided into four main parts:

- development of derived constraints (Sections 6.2 and 6.6),
- deterministic analysis (Section 6.3),
- analysis of barrier effectiveness (Section 6.4), and
- probabilistic analysis (Section 6.5).

Sections 6.7 and 6.8 discuss the analyses for the open-borehole and inadvertent human intrusion scenarios respectively.

The following paragraphs introduce and put into context the material in Sections 6.2 to 6.8.

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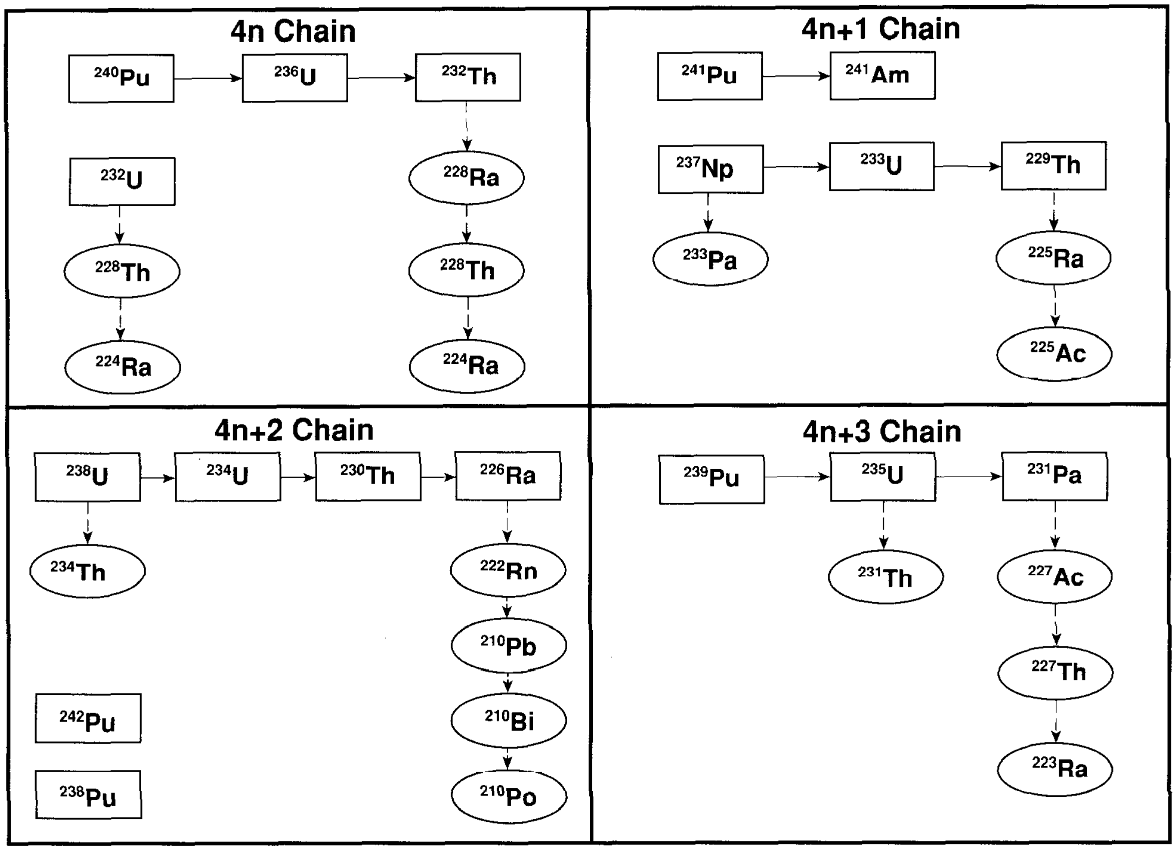

FIGURE 5-22: Abbreviated Form of the Four Actinide Decay Chains

This figure illustrates the scheme used in simulating the four actinide decay chains. The actinides are a group of chemical elements with atomic numbers from 89 to 103, all of which are radioactive. Long-lived actinides include ^{237}Np, ^{239}Pu, ^{238}U and ^{232}Th. The formulae 4n, 4n+1, 4n+2 and 4n+3 give the mass numbers of members in a chain, where n is an integer. The original actinide decay chains contain more than 75 radionuclides, but only 33 need be included in the system model for the reference disposal system (Goodwin and Mehta 1994). (The figure contains 35 entries because ^{224}Ra and ^{228}Th both appear twice.)

- A radionuclide enclosed in a rectangle is represented explicitly in the models for the vault, geosphere and biosphere. The solid arrows show how such radionuclides are connected within a decay chain; for example, the modelling of ^{236}U in the 4n decay chain explicitly includes losses in its mass from its decay to ^{232}Th, and increases in its mass, because of ingrowth from the decay of ^{240}Pu.

- A radionuclide enclosed in an oval is not modelled in the vault and geosphere models, nor in the overburden and lake sediment because its concentrations can be estimated from the concentration of its precursor radionuclide(s), using an approximation known as secular equilibrium (see text). They are modelled explicitly in the biosphere model, except in the food-chain model that also uses the secular-equilibrium approximation. The dashed arrows identify precursor radionuclides; for example, the precursor to ^{224}Ra is ^{228}Th, and the precursors to ^{228}Th are ^{232}U and ^{228}Ra.

Note that all radionuclides in this figure are included in the food-chain component of the biosphere model, which calculates the annual dose estimates to members of the critical group (Davis et al. 1993).

Development of Derived Constraints

When selecting and developing an actual disposal system, it would be generally possible to derive constraints pertaining to the location and design of the vault so as to increase the expected margin of safety. We demonstrate in Section 6.2 how preliminary assessments can be used to develop effective derived constraints, and thus provide an avenue for refining the design of a facility for a particular site.

The studies described in Section 6.2 are based on a deterministic analysis. The resultant derived constraints are used to revise the design of the reference disposal system, and this revised system is then analyzed in Sections 6.3 to 6.5.

Section 6.6 continues the discussion of derived constraints. It uses a probabilistic analysis to illustrate how the postclosure assessment could be used to provide more information on some potential design features. Section 6.6 also studies the effects of assumed changes to selected site features.

Deterministic Analysis

Section 6.3 deals with a deterministic analysis, that is, the study of a single simulation in which all parameters are given known values. We have chosen for analysis one particular simulation that is representative of central tendencies. It is known as the median-value simulation because the value selected for each parameter is its median value. The median value of a parameter is the middle or central value of its PDF. More precisely, if its PDF were sampled randomly, the sampled value would be bigger than the median with a probability of 0.5 and smaller than the median with the same probability. Sensitivity analysis of the median-value simulation is also discussed in Section 6.3. Appendix D provides more details on the analysis of the median-value simulation.

The deterministic analysis is focussed mostly on annual dose estimates (ADEs) to members of the critical group, with some discussion of ADEs to nonhuman biota and concentrations of chemically toxic elements. We document the deterministic analysis in this report for two main reasons:

- It provides more detail and insight into the operation and interactions of the system model than is possible in the probabilistic analysis. For example, the simulation results can describe the failure of the containers, the release of contaminants from the waste matrices and the subsequent movement of contaminants throughout the disposal system.

- Sensitivity analysis of the results further improves our understanding of important factors and subtle effects. This is particularly useful in supplementing the probabilistic analysis described below. Our experience has shown that probabilistic analysis that considers only a set of randomly sampled simulations is likely to identify just a few of the most important effects and interactions because more subtle effects tend to be obscured by the variations in parameter values.

Analysis of Barrier Effectiveness

Section 6.4 describes a special sensitivity analysis to examine the relative effectiveness of the engineered and natural barriers that contribute to the safety of the reference disposal system. It studies the main barriers along the pathway that contribute most to ADEs in the deterministic analysis.

The barriers studied are the titanium container, used fuel and Zircaloy waste matrices, buffer, backfill, precipitation in the buffer, the rock within the waste exclusion distance, and two parts of fracture zone LD1 that extend from near the vault horizon to the well used by the critical group. The analysis examines the effectiveness of each barrier for different contaminants and examines how the effectiveness changes with time. It also shows how the sequence of independent barriers contribute to produce a disposal system having a large margin of safety.

Probabilistic Analysis

Section 6.5 describes the probabilistic analysis using the results from more than 40 000 simulations in which parameter values are randomly selected from their probability distributions. Sensitivity analysis of the probabilistic simulations is also discussed in Section 6.5. Appendix E provides more details.

We use the results of the probabilistic analysis for comparison with regulatory criteria. We note in Chapter 2 that the strength of probabilistic analysis is its ability to take into account the effects of parameter uncertainties. We show that uncertainties can have a strong influence on the results of such an assessment and, therefore, we use the probabilistic approach to obtain the estimates for important performance measures, such as

- average annual dose to members of the critical group and to nonhuman biota, and
- average concentrations of chemically toxic contaminants in the local habitat of the critical group and other biota.

We also perform a probabilistic sensitivity analysis of the system model to identify important parameters, pathways and contaminants in the disposal system when uncertainty of all parameters is taken into consideration.

Analysis of the Open-Borehole and Inadvertent Human Intrusion Scenarios

Scenario analysis for the reference disposal system (Chapter 4) has identified three types of scenarios requiring quantitative evaluation for times up to 10^4 a.

- Sections 6.2 to 6.6 deal with the SYVAC scenarios, which collectively describe the expected behaviour of the disposal system through groundwater-mediated processes.

- Sections 6.7 deals with the analysis of the open-borehole scenarios, which describe an unlikely situation in which one or more open boreholes pass near the reference disposal vault.

- Section 6.8 deals with the low-probability inadvertent human intrusion scenarios in which the integrity of the reference disposal system might be seriously disrupted by exploratory drilling.

6.2 STUDY OF DERIVED CONSTRAINTS

6.2.1 Development of Design Constraints for the Reference System

The studies described in this section refer to an interim design of the reference disposal system. As discussed below, the interim design differs from the final design evaluated in the remainder of this chapter with respect to the layout of the vault relative to fracture zone LD1.

For our studies, we assume that a hypothetical disposal vault is located at a depth of 500 m in plutonic rock of the Canadian Shield. In constructing the interim design for the reference disposal system, we based its geological and hydrological characteristics on information from the WRA, including the URL in the WRA, as discussed in Chapter 5. However, we refer to the corresponding studies as preliminary analyses because they used preliminary versions of the models and data.

Although these preliminary models and data resemble closely those described in Chapter 5 and used in the following sections of Chapter 6, some changes have since been implemented, the most notable being the adoption of one particular design constraint (discussed below). Design constraints are restrictions on the disposal system design. Examples of possible restrictions are the thickness of the buffer material, the type of container material or the layout of vault rooms relative to nearby geological features. These restrictions are referred to as derived constraints because they follow from an analysis of impacts, and not directly from regulatory criteria.

In Sections 6.2.2 and 6.2.3, we outline our preliminary analyses of potential design constraints. One particular constraint was very effective in reducing predicted annual doses from the reference disposal system. We used this constraint to develop the "final" design of the reference disposal system. This design is final in the sense that it is the one that is subsequently evaluated and documented in Sections 6.3 to 6.5. Further assessment studies could lead to more modifications to the reference disposal system and, almost certainly, there would be a different design for a disposal facility at some other site.

The development and application of derived constraints is another example of the feedback in the method developed for the postclosure assessment (Figure 2-1).

6.2.2 Results from Design Constraint Studies

A number of potential design constraints were examined to identify those that would be effective in improving the performance of the reference disposal system. They included

- A thicker layer of buffer between the container and surrounding rock. The extra thickness would increase the time required for diffusion of contaminants from the container to the surrounding media.

- Titanium containers with thicker walls. The extra thickness would increase the time for corrosion processes to breach the container.

- More durable container material. Current evidence indicates that very long-lived containers could be fabricated from a variety of materials, including copper and titanium (King and LeNeveu 1992, Ikeda et al. 1994).

The effects of these constraints were as expected: each led to smaller ADEs. The third constraint, a more durable container, could be much more significant in reducing ADEs. In each case, the smaller ADEs occur because the constraints act to delay the release or rate of transport of radionuclides. These reduced annual doses are observed over the 10^5-year time period of the simulations. However, because the major contributor to dose is ^{129}I, and because ^{129}I has a long half-life, the reductions would tend to become less significant at longer times.

Another design constraint led to even more significant improvement in the performance of the disposal system:

- Modify the layout of the vault to provide greater isolation from a nearby geological feature, fracture zone LD1.

We considered several different options related to vault layout. The starting point was the vault described in the conceptual design study, (Simmons and Baumgartner 1994); it measures approximately 2000 m by 2000 m and contains 191 000 Mg U. The three main options considered were to

- move the vault (2000 x 2000 m) farther away from fracture zone LD1;

- adjust the vault dimensions to a rectangular arrangement in which the vault rooms closest to LD1 are moved out to the sides, away from LD1; and

- eliminate all or parts of some vault rooms nearest LD1.

In our detailed analysis, we chose the third option to take advantage of the detailed geological and hydrological information that was available.

We examined two aspects of this design constraint related to the layout of the vault for the reference disposal system. They are illustrated in Figure 6-1 and relate to

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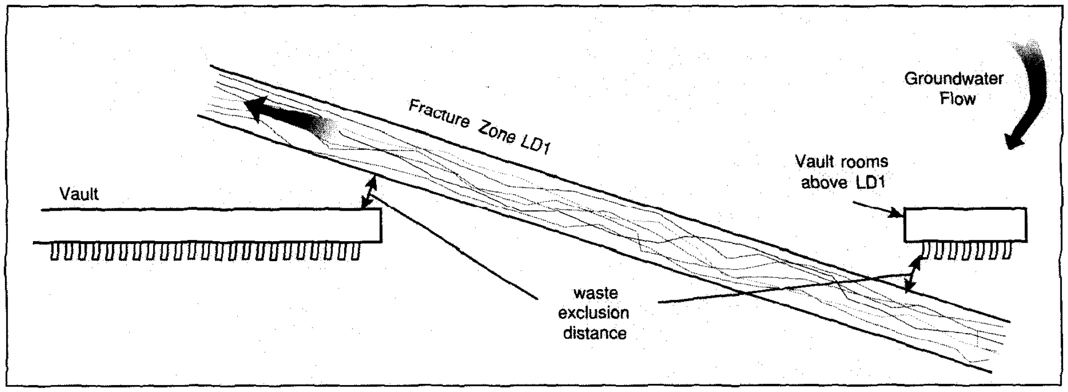

FIGURE 6-1: A Design Constraint Applied to the Layout of the Vault

We examine two aspects of this design constraint for an interim design of a hypothetical vault located at a depth of 500 m and having a set of geological and hydrological properties similar to those of the WRA. Our analysis shows that substantial improvements in performance can be achieved

- by increasing the waste exclusion distance that separates the waste emplacement part of any vault room from fracture zone LD1, and

- by eliminating all vault rooms located above fracture zone LD1.

We have adopted these constraints to develop a final design for the reference disposal system.

- *The waste exclusion distance.* In Section 5.2, we note there is a zone of low permeability within the waste exclusion distance that isolates the containers in the vault rooms nearest to fracture zone LD1. In the chosen option, a 50-m waste exclusion distance is achieved by eliminating all or part of the vault rooms nearest the fracture zone.

- *Elimination of all vault rooms located above fracture zone LD1.* Groundwater velocities are considerably higher in the rock above fracture zone LD1 compared with the rock below LD1.

Our analysis shows that both a larger waste exclusion distance and no rooms above fracture zone LD1 would lead to much smaller ADEs. For example, in simulations in which all parameters are given their median values, we find that

- Increasing the waste exclusion distance from about 30 m to about 50 m reduces ADEs from ^{129}I by 13 orders of magnitude at 10^4 a and by almost 1 order of magnitude at 10^5 a. The reduction in dose is mostly due to the increased transport time of contaminants through the greater thickness of sparsely fractured rock; the associated reduction in inventory has a much smaller effect.

- Removing vault rooms from above LD1 reduces estimated annual doses from ^{129}I by almost 6 orders of magnitude at 10^4 a and 2 orders of magnitude at 10^5 a. This reduction in dose occurs because groundwater flow velocities above LD1 are more than 10 times faster than flow velocities below LD1, leading to much more rapid contaminant transport. Moreover, flow velocities above LD1 are directed downwards so that contaminants leaving the buffer from rooms above LD1 would pass directly into the rock, without passing through any part of the backfill (see Figures 6-1 and 5-9). The backfill acts to further delay contaminant transport.

- Similar effects are observed for other radionuclides, such as ^{14}C and ^{99}Tc. Estimated doses from ^{14}C are attenuated even more because of radioactive decay (it has a shorter half-life of 5730 a). Estimated doses from ^{99}Tc are especially attenuated when the backfill lies in its flow path because ^{99}Tc is strongly sorbed onto the mixture of clay and crushed rock making up the backfill.

The reductions in ADEs are greatest at earlier times but tend to become less significant at longer times. This is because the major contributor to dose is long-lived ^{129}I: at early times its breakthrough is just starting, whereas at times near 10^5 a its breakthrough has more closely approached a psuedo steady-state value that is not significantly reduced by radioactive decay. Section 6.6 and Section E.8 in Appendix E provide further analyses on the effects of different waste exclusion distances.

With a waste exclusion distance of about 50 m and no vault rooms above LD1, the length and width of the vault for the reference disposal system are approximately 1900 m and 1700 m respectively. We assume that there is the same density of containers per unit length of a vault room as in the conceptual vault design (Simmons and Baumgartner 1994), and thus the inventory for the reference disposal system is reduced to 162 000 Mg U. This reduced inventory is a result of the option chosen to achieve the 50-m exclusion distance and does not indicate a limit to the capacity of the reference disposal system (or any other disposal system).

The data cited above are obtained from the detailed layout drawings of the vault relative to fracture zone LD1. These drawings also provide a more precise value of 46.5 m for the waste exclusion distance. Although the system model for the reference disposal system uses these more precise values, we have not conducted a thorough optimization study. Thus we refer to a waste exclusion distance of *about* 50 m in this document.

6.2.3 Conclusions: Changes to the Reference Disposal System

We used the results of the preliminary studies of derived constraints to modify the design of the reference disposal system used in this postclosure assessment study. In the modified design, we assume

- the waste exclusion distance is about 50 m, and

- there are no vault rooms located above fracture zone LD1.

With these constraints, the reference disposal vault considered in the following sections is about 1900 by 1700 m, and it contains 162 000 Mg U.

As noted above, these particular constraints are specific to the reference disposal system that is based on geological and hydrological information from the WRA and that is located at a depth of 500 m. The approach used, however, illustrates the analysis that would be used to derive constraints that might be applied during the planning and construction of an actual disposal facility, using information from postclosure assessment studies.

6.3 RESULTS FROM THE MEDIAN-VALUE SIMULATION

6.3.1 Introduction to the Median-Value Simulation

In the single simulation performed for the deterministic analysis, all model parameters are given their median values (the middle value or 50^{th} percentile of their PDFs). We analyze this simulation to identify important features and processes (and to explain why they are important) in the system model and to observe some relatively subtle effects that are difficult to distinguish in the results from the many randomly selected simulations. We believe that the results of the probabilistic analysis (Section 6.5) are more suitable for comparing estimated impacts with regulatory criteria.

In the system model, we simulate the movement of contaminants out of the waste matrices, through the engineered barriers of the vault and the natural rock barrier, and into the biosphere where they lead to estimated impacts on the critical group and other biota. The results indicate that very small amounts of contaminants would be released to the environment over the period up to 10^4 a after closure.

In fact, we estimate very small amounts would be released over 10^5 a after closure. Most of our results are discussed over 10^5 a, even though the AECB radiological risk criterion pertains to only the first 10^4 a after closure of the disposal vault. We consider the longer time frame to show the projected trends in the reference disposal system.

Section 5.9 lists the contaminants represented in the median-value simulation; they include 68 radionuclides and 9 chemically toxic elements. Some of these contaminants are present both in used fuel and in Zircaloy sheaths; we model them separately as they have different inventories and rates of release. For instance, ^{14}C is about 5 times more abundant in used fuel than in Zircaloy (Section 5.9) and its release from the used-fuel matrix includes the instant-release mechanism (Section 5.2).

Much of the discussion is focussed on ^{129}I and ^{14}C from the used-fuel matrix because these two radionuclides are by far the most important in determining the ADEs for the median-value simulation. As we show later, they are also the most important to the ADE in the probabilistic analysis. However, we include discussion on ^{99}Tc, the ^{238}U decay chain and some other contaminants to illustrate their behaviour and movement throughout the disposal system. The discussion of ^{99}Tc describes the effects of contaminant precipitation in the vault, and the analysis of the ^{238}U decay series illustrates the effects of a decay chain on contaminant inventories in waste matrices and barriers. Uranium-238 is also included because it is the most abundant radionuclide in used fuel.

The following discussion presents an overview of the results of the median-value simulation. Appendix D contains more detailed results of the analysis, including an examination of intermediate results from the vault, geosphere and biosphere models.

6.3.2 Overview of the Results

Figure 6-2 shows the flow path for the median-value simulation that leads to the largest radiological impacts on members of the critical group. Contaminants move

- From the waste matrices, containers, buffer and backfill in vault sector 11 into the surrounding rock;
- Through the rock within the waste exclusion distance (about 50 m long) to fracture zone LD1;
- Along the fracture zone to its intersection with the well; and
- Into the local environment of the critical group. Members of the critical group are affected mainly through ingestion of plants that have been irrigated with well water, animal products from domestic animals that drink the well water, and through direct ingestion of well water. Other organisms would also be affected through contamination of the air, soil and water of the biosphere.

Contaminant transport is mostly controlled by diffusion in the vault and in the rock within the waste exclusion distance. Once in fracture zone LD1, contaminant transport in moving groundwater is more important than transport by diffusion.

Figure 6-3 shows the ADE versus time for the median-value simulation. At 10^4 a after closure, the ADE is 3×10^{-18} Sv/a, and it rises to 4×10^{-7} Sv/a by 10^5 a. These doses are barely visible in curve (a) of Figure 6-3, which has been scaled to show the annual dose, 5×10^{-5} Sv/a, associated with the AECB risk criterion, and which is prescribed for times up to 10^4 a following closure (AECB 1987a). For comparison, total annual dose from radiation in the natural environment is about 3×10^{-3} Sv/a.

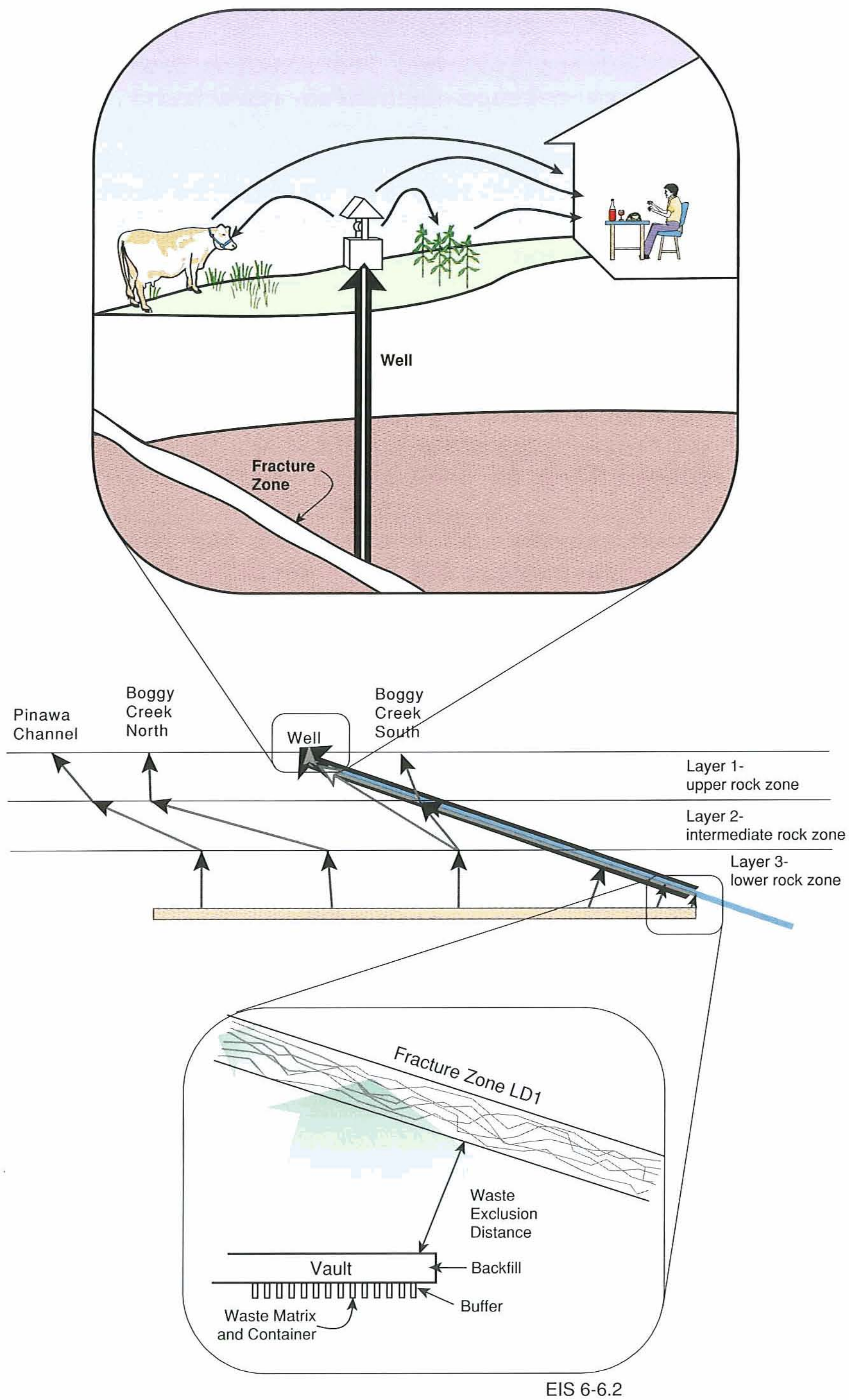

FIGURE 6-2: Principal Flow Path Leading from the Vault to Members of the Critical Group

For the median-value simulation, contaminants move from vault sector 11 through the waste exclusion distance (about 50 m of sparsely fractured rock) to fracture zone LD1, and then upwards along LD1 to its intersection with the well. The contaminants would affect members of the critical group mainly through ingestion of fruit, berries and vegetables grown on a garden irrigated with well water, through ingestion of animal products from animals that drink the well water, and through direct ingestion of well water.

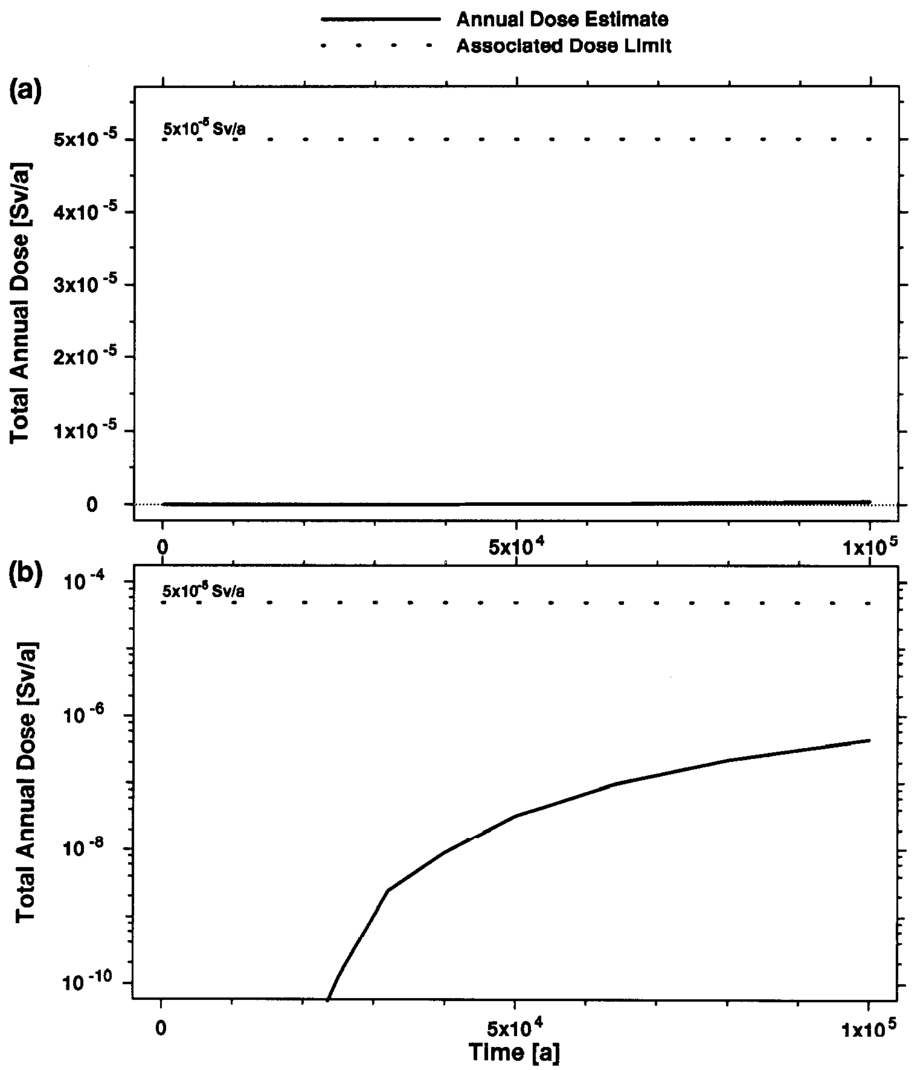

FIGURE 6-3: Estimated Total Annual Dose for the Median-Value Simulation

These curves show the annual dose estimates (ADEs) from all radionuclides to an individual in the critical group. Both curves use the same data but different vertical axes: curve (a) uses a linear axis; and curve (b), a logarithmic axis. Both vertical axes are scaled to show the annual dose of 5×10^{-5} Sv/a associated with the AECB radiological risk criterion, which pertains to a time frame of 10^4 a (AECB 1987a). The starting point (time equal to zero) is the time of closure of the vault, and the curves are extended to the time limit of the simulations (10^5 a).

The results indicate that ADEs are very small over the entire simulation time. The estimated annual dose reaches a maximum of 4×10^{-7} Sv/a at 10^5 a. This maximum is less than 1% of the dose associated with the risk criterion and less than 0.05% of the annual dose from natural background. Simulation results extrapolated to even longer time-scales show a peak in the ADE occurring near 10^6 a that is less than 5×10^{-5} Sv/a.

Figure 6-4 is a plot of the ADE versus time that includes additional curves showing the total dose and the contributions from each of several individual radionuclides. The curve for total annual dose represents the sum of the contributions from all 68 radionuclides identified in Table 5-4. Of these radionuclides, only ^{129}I, ^{81}Kr and ^{14}C are discharged to the biosphere in appreciable quantities in 10^5 a (Table 6-1). Figure 6-4 illustrates clearly that ^{129}I is the only major contributor to dose at all times up to 10^5 a. Carbon-14 from used fuel contributes at most 0.1% to the total. (Recent experimental data for instant-release fractions indicate that this contribution from ^{14}C is significantly overestimated. Other data indicates there may be significant contributions from ^{36}Cl. Section 8.2.6 provides more discussion on these issues.) Carbon-14 from Zircaloy also appears on the plot, but its ADEs are much smaller because ^{14}C release rates are much smaller from Zircaloy than from used fuel. Krypton-81 does not appear in the plot because krypton is a noble gas and its contribution to dose is only through external exposure, an unimportant exposure route for the reference disposal system (because of the small concentrations of ^{81}Kr that are estimated for all parts of the biosphere). Not shown are curves for other contaminants, such as ^{239}Pu and ^{99}Tc from used fuel, and ^{208}Bi from Zircaloy; their ADEs are more than 14 orders of magnitude smaller than those for ^{129}I.

Table 6-1 summarizes the fate of the 68 radionuclides and 9 chemically toxic elements for the median-value simulation. It shows, at 10^5 a, the estimated amounts of each contaminant at selected locations in the reference disposal system. At this time, most of the contaminants remain in the vault, contained within the used fuel or Zircaloy matrices. Only a few contaminants reach the geosphere, and fewer still discharge to the biosphere in any appreciable quantities. Table 6-1 shows the total amounts discharged to the biosphere, over 10^5 a, exceed a small value of 10^{-15} mol for only

- the chemically toxic elements bromine and antimony (from used fuel); and

- the radionuclides ^{14}C (from both used fuel and Zircaloy), ^{129}I (used fuel) and ^{81}Kr (used fuel).

Table 6-1 also indicates the effects of radioactive decay and ingrowth. Many radioactive contaminants show a decline in inventory. For example, there is no ^{39}Ar remaining in the vault, geosphere and biosphere at 10^5 a, because its half-life is only 269 a and its initial inventory will have essentially disappeared. Longer-lived radionuclides, such as ^{129}I (half-life, 1.57×10^7 a), show very little decrease in inventory. Finally, some members of decay chains may actually increase in inventory because of ingrowth from their precursors. This is the case for ^{231}Pa. Its initial inventory is 2.2×10^{-2} mol, but the amount in the vault by 10^5 a increases to approximately 1.2×10^2 mol because of ingrowth from its two precursors, ^{239}Pu and ^{235}U, shown in Figure 5-22.

Figures 6-5 to 6-8 show the distributions of ^{129}I, ^{14}C, ^{99}Tc and ^{238}U throughout the disposal system after periods of 10^4 a and 10^5 a following closure. The results indicate the effectiveness of the engineered and

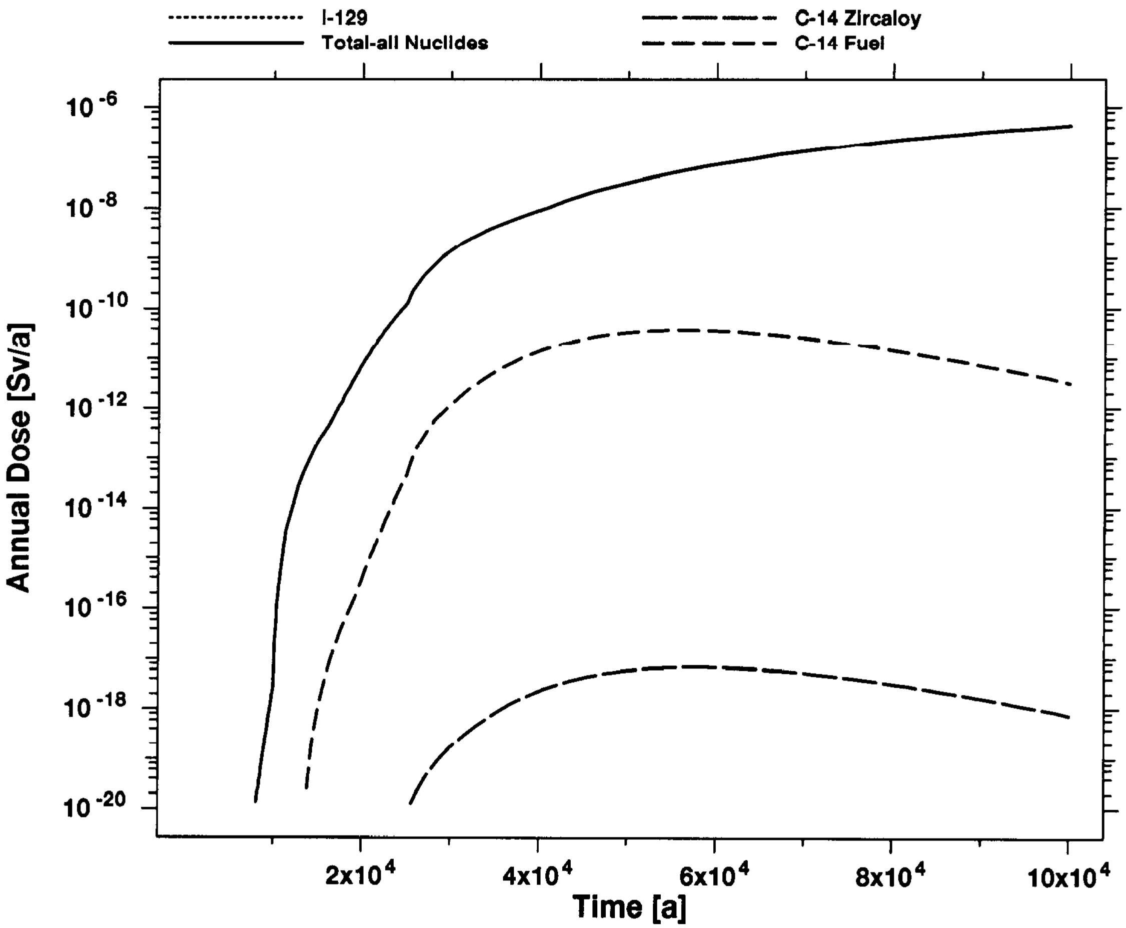

FIGURE 6-4: Contributors to Estimated Annual Dose for the Median-Value Simulation

The topmost curve in this figure is the same as that in (b) of Figure 6-3: both show the total annual dose estimate (ADE) to an individual in the critical group as a function of time. This figure also shows the relative importance of the three largest contributors to the ADE. The largest contributor is ^{129}I; in fact, the curve of its ADE coincides with the curve for total ADE. The next largest contributor is ^{14}C from used fuel; it contributes up to 1 part in 10^3 to the total. The third largest contributor is ^{14}C from Zircaloy, but it contributes less than 1 part in 10^9 to the total. All other radionuclides in Table 5-4 make even smaller contributions than ^{14}C from Zircaloy.

TABLE 6-1

FATE* OF CONTAMINANTS AT 10^5 a

Radio-Nuclide or Toxic Element**	Initial Inventory (mol)	Amount in Containers at 10^5 a (mol)	Amount in Buffer at 10^5 a (mol)	Amount in Backfill at 10^5 a (mol)	Amount in Vault at 10^5 a (mol)	Vault Release to 10^5 a (mol)	Amount in Geosphere at 10^5 a (mol)	Amount Released to Biosphere at 10^5 a (mol)
^{241}Am	5.9×10^{4}	0.0	0.0	0.0	0.0	0.0	0.0	0.0
^{39}Ar	3.3×10^{-2}	0.0	0.0	0.0	0.0	1.6×10^{-10}	0.0	$<10^{-20}$
^{10}Be	1.4×10^{-1}	1.3×10^{-1}	0.0	5.0×10^{-13}	1.3×10^{-1}	8.5×10^{-10}	8.3×10^{-10}	0.0
^{10}Be Z	2.7×10^{-2}	2.6×10^{-2}	0.0	3.6×10^{-12}	2.6×10^{-2}	6.2×10^{-9}	6.0×10^{-9}	0.0
^{208}Bi Z	1.6×10^{-5}	1.3×10^{-5}	3.0×10^{-12}	4.4×10^{-14}	1.3×10^{-5}	2.0×10^{-16}	1.9×10^{-16}	$<10^{-20}$
^{210m}Bi Z	2.3×10^{-4}	2.3×10^{-4}	5.2×10^{-11}	7.7×10^{-13}	2.3×10^{-4}	3.4×10^{-15}	3.4×10^{-15}	7.4×10^{-20}
Br	1.1×10^{4}	9.9×10^{3}	0.0	5.9×10^{2}	1.1×10^{4}	9.8×10^{1}	9.8×10^{1}	2.4×10^{-2}
^{14}C	3.0×10^{3}	1.5×10^{-2}	0.0	1.6×10^{-3}	1.6×10^{-2}	1.8	2.6×10^{-4}	8.1×10^{-7}
^{14}C Z	5.3×10^{2}	2.9×10^{-3}	0.0	6.5×10^{-10}	2.9×10^{-3}	3.5×10^{-7}	8.0×10^{-11}	1.5×10^{-13}
^{41}Ca	2.1×10^{2}	1.3×10^{2}	0.0	5.0×10^{-10}	1.3×10^{2}	1.1×10^{-6}	8.1×10^{-7}	0.0
Cd	1.9×10^{4}	1.9×10^{4}	4.6×10^{-6}	1.0×10^{-5}	1.9×10^{4}	1.0×10^{-4}	1.0×10^{-4}	0.0
^{113m}Cd	2.8×10^{1}	0.0	0.0	0.0	0.0	1.4×10^{-16}	0.0	0.0
Cr Z	3.5×10^{5}	3.5×10^{5}	0.0	5.1×10^{-5}	3.5×10^{5}	8.1×10^{-2}	8.1×10^{-2}	0.0
Cs	6.8×10^{5}	6.2×10^{5}	0.0	0.0	6.2×10^{5}	5.6×10^{4}	5.6×10^{4}	0.0
^{135}Cs	2.8×10^{4}	2.5×10^{4}	0.0	0.0	2.5×10^{4}	2.3×10^{3}	2.3×10^{3}	0.0
^{3}H	4.5×10^{2}	0.0	0.0	0.0	0.0	1.8×10^{-10}	0.0	0.0
^{3}H Z	5.2×10^{-3}	0.0	0.0	0.0	0.0	$<10^{-20}$	0.0	0.0
^{182}Hf Z	3.6	3.5	6.1×10^{-7}	2.1×10^{-7}	3.5	5.8×10^{-16}	5.8×10^{-16}	0.0
^{129}I	5.6×10^{4}	5.2×10^{4}	0.0	3.1×10^{3}	5.5×10^{4}	5.2×10^{2}	5.2×10^{2}	2.8×10^{-1}
^{40}K	3.6×10^{1}	3.3×10^{1}	3.9×10^{-1}	2.5	3.6×10^{1}	7.2×10^{-2}	7.2×10^{-2}	0.0

continued...

TABLE 6-1 (continued)

Radio-Nuclide or Toxic Element**	Initial Inventory (mol)	Amount in Containers at 10^5 a (mol)	Amount in Buffer at 10^5 a (mol)	Amount in Backfill at 10^5 a (mol)	Amount in Vault at 10^5 a (mol)	Vault Release to 10^5 a (mol)	Amount in Geosphere at 10^5 a (mol)	Amount Released to Biosphere at 10^5 a (mol)
^{81}Kr	1.1×10^{-2}	7.2×10^{-3}	6.8×10^{-5}	5.0×10^{-4}	7.7×10^{-3}	8.6×10^{-5}	7.5×10^{-5}	1.3×10^{-8}
^{85}Kr	6.0×10^{3}	0.0	0.0	0.0	0.0	3.6×10^{-10}	0.0	0.0
Mo	1.3×10^{6}	1.3×10^{6}	8.3×10^{-3}	1.6×10^{-5}	1.3×10^{6}	2.4×10^{-14}	2.4×10^{-14}	$<10^{-20}$
^{93}Mo	2.6×10^{-1}	6.6×10^{-10}	7.0×10^{-18}	1.2×10^{-20}	6.6×10^{-10}	$<10^{-20}$	$<10^{-20}$	0.0
^{93}Mo Z	4.1×10^{-1}	1.0×10^{-9}	4.0×10^{-16}	6.7×10^{-19}	1.0×10^{-9}	$<10^{-20}$	$<10^{-20}$	0.0
^{94}Nb Z	1.0×10^{2}	3.4	5.9×10^{-7}	2.1×10^{-7}	3.4	7.3×10^{-16}	5.5×10^{-16}	0.0
^{59}Ni	5.7×10^{2}	2.3×10^{2}	0.0	9.1×10^{-10}	2.3×10^{2}	2.7×10^{-6}	1.4×10^{-6}	0.0
^{59}Ni Z	1.6×10^{2}	6.5×10^{1}	0.0	9.6×10^{-9}	6.5×10^{1}	2.9×10^{-5}	1.5×10^{-5}	0.0
^{63}Ni	9.7×10^{1}	0.0	0.0	0.0	0.0	4.1×10^{-13}	0.0	0.0
^{63}Ni Z	2.8×10^{1}	0.0	0.0	0.0	0.0	4.4×10^{-12}	0.0	0.0
^{237}Np	1.8×10^{5}	1.8×10^{5}	1.1×10^{-3}	2.2×10^{-6}	1.8×10^{5}	3.2×10^{-15}	3.2×10^{-15}	0.0
^{231}Pa	2.2×10^{-2}	1.2×10^{2}	8.2×10^{-7}	1.3×10^{-7}	1.2×10^{2}	1.3×10^{-16}	1.1×10^{-16}	0.0
^{205}Pb Z	3.7×10^{-1}	3.7×10^{-1}	0.0	1.7×10^{-10}	3.7×10^{-1}	8.6×10^{-8}	8.6×10^{-8}	0.0
^{107}Pd	8.2×10^{4}	8.1×10^{4}	5.1×10^{-5}	9.2×10^{-5}	8.1×10^{4}	3.7×10^{-4}	3.6×10^{-4}	0.0
^{238}Pu	3.3×10^{3}	0.0	0.0	0.0	0.0	0.0	0.0	0.0
^{239}Pu	1.9×10^{6}	1.0×10^{5}	4.8×10^{-4}	1.7×10^{-4}	1.0×10^{5}	5.8×10^{-13}	4.5×10^{-13}	0.0
^{240}Pu	6.9×10^{5}	1.7×10^{1}	8.4×10^{-8}	2.9×10^{-8}	1.7×10^{1}	2.4×10^{-16}	7.5×10^{-17}	0.0
^{241}Pu	9.6×10^{4}	0.0	0.0	0.0	0.0	0.0	0.0	0.0
^{242}Pu	4.0×10^{4}	3.4×10^{4}	1.6×10^{-4}	5.4×10^{-5}	3.4×10^{4}	1.5×10^{-13}	1.5×10^{-13}	0.0
^{226}Ra	4.3×10^{-5}	1.3×10^{2}	9.8×10^{-7}	3.0×10^{-8}	1.3×10^{2}	3.4×10^{-6}	1.9×10^{-7}	0.0

continued...

TABLE 6-1 (continued)

Radio-Nuclide or Toxic Element**	Initial Inventory (mol)	Amount in Containers at 10^5 a (mol)	Amount in Buffer at 10^5 a (mol)	Amount in Backfill at 10^5 a (mol)	Amount in Vault at 10^5 a (mol)	Vault Release to 10^5 a (mol)	Amount in Geosphere at 10^5 a (mol)	Amount Released to Biosphere at 10^5 a (mol)
^{87}Rb	1.0×10^5	9.4×10^4	8.0×10^3	3.8×10^2	1.0×10^5	1.6	1.6	0.0
^{187}Re Z	4.4×10^2	4.4×10^2	1.0×10^{-4}	2.0×10^{-7}	4.4×10^2	2.9×10^{-16}	2.9×10^{-16}	$<10^{-20}$
Sb	3.2×10^3	3.2×10^3	2.0×10^{-5}	2.9×10^{-7}	3.2×10^3	1.3×10^{-9}	1.3×10^{-9}	3.0×10^{-14}
^{125}Sb	3.0×10^2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
^{125}Sb Z	1.8×10^1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Se	2.6×10^4	2.4×10^4	0.0	0.0	2.4×10^4	1.7×10^3	1.7×10^3	0.0
^{79}Se	2.7×10^3	8.5×10^2	0.0	0.0	8.5×10^2	1.5×10^2	5.9×10^1	0.0
^{32}Si	2.5×10^{-6}	0.0	0.0	0.0	0.0	0.0	0.0	0.0
^{32}Si Z	6.3×10^{-7}	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Sm	2.4×10^5	2.4×10^5	1.1×10^{-3}	3.8×10^{-4}	2.4×10^5	1.0×10^{-12}	1.0×10^{-12}	0.0
^{126}Sn	6.3×10^3	2.9×10^3	0.0	0.0	2.9×10^3	5.1×10^2	2.6×10^2	0.0
^{90}Sr	1.8×10^5	0.0	0.0	0.0	0.0	1.1×10^{-4}	0.0	0.0
Tc	3.3×10^5	2.3×10^5	1.5×10^4	1.2×10^{-1}	2.4×10^5	1.7×10^{-10}	1.7×10^{-10}	$<10^{-20}$
^{99}Tc	3.3×10^5	2.3×10^5	1.5×10^4	1.2×10^{-1}	2.4×10^5	1.7×10^{-10}	1.7×10^{-10}	$<10^{-20}$
^{99}Tc Z	4.3	3.1	7.1×10^{-7}	1.4×10^{-9}	3.1	2.1×10^{-18}	2.1×10^{-18}	0.0
^{229}Th	5.2×10^{-6}	2.0×10^2	1.2×10^{-6}	5.4×10^{-8}	2.0×10^2	1.2×10^{-16}	7.2×10^{-17}	0.0
^{230}Th	8.9×10^{-1}	6.3×10^3	4.8×10^{-5}	9.8×10^{-6}	6.3×10^3	1.1×10^{-14}	1.1×10^{-14}	0.0
^{232}Th	1.6×10^{-1}	3.4×10^3	5.8×10^{-3}	1.9×10^{-3}	3.4×10^3	3.5×10^{-12}	3.5×10^{-12}	0.0
^{232}U	2.9×10^{-2}	0.0	0.0	0.0	0.0	0.0	0.0	0.0
^{233}U	1.5×10^{-1}	4.7×10^3	2.9×10^{-5}	5.7×10^{-8}	4.7×10^3	1.1×10^{-15}	1.0×10^{-15}	0.0

continued...

TABLE 6-1 (concluded)

Radio-Nuclide or Toxic Element**	Initial Inventory (mol)	Amount in Containers at 10^5 a (mol)	Amount in Buffer at 10^5 a (mol)	Amount in Backfill at 10^5 a (mol)	Amount in Vault at 10^5 a (mol)	Vault Release to 10^5 a (mol)	Amount in Geosphere at 10^5 a (mol)	Amount Released to Biosphere at 10^5 a (mol)
^{234}U	3.3×10^{4}	3.4×10^{4}	2.1×10^{-4}	4.1×10^{-7}	3.4×10^{4}	2.0×10^{-15}	2.0×10^{-15}	0.0
^{235}U	1.4×10^{5}	3.1×10^{6}	2.5×10^{-2}	3.7×10^{-4}	3.1×10^{6}	7.3×10^{-14}	1.9×10^{-13}	0.0
^{236}U	5.3×10^{5}	1.2×10^{6}	8.5×10^{-3}	2.3×10^{-5}	1.2×10^{6}	2.7×10^{-14}	2.7×10^{-14}	0.0
^{238}U	6.7×10^{8}	6.7×10^{8}	4.2	8.3×10^{-3}	6.7×10^{8}	1.2×10^{-11}	1.2×10^{-11}	0.0
^{93}Zr	2.9×10^{5}	2.8×10^{5}	1.3×10^{-3}	4.5×10^{-4}	2.8×10^{5}	1.2×10^{-12}	1.2×10^{-12}	0.0
^{93}Zr Z	3.2×10^{4}	3.0×10^{4}	5.2×10^{-3}	1.8×10^{-3}	3.0×10^{4}	4.9×10^{-12}	4.9×10^{-12}	0.0

* This table shows the calculated location of the contaminants at 10^5 a for the median-value simulation. The first column identifies the radionuclides and nine chemically toxic elements, and the second column lists their initial inventories. Columns 3, 4 and 5 give the amounts in the containers (including the used-fuel and Zircaloy waste matrices), buffer and backfill at 10^5 a. These amounts are summed in column 6, for the amounts in the vault. Column 7 lists the total amounts released from the vault for times up to 10^5 a. The last two columns describe the total amounts in the geosphere at 10^5 a and the total amounts discharged to the biosphere over 10^5 a. Entries of 0.0 indicate that the calculated value is less than 10^{-37} (a number related to precision of the computer).
At 10^5 a, most of the contaminants remain within the vault. Total discharges over 10^5 a to the biosphere exceed 10^{-15} mol only for Br, ^{14}C, ^{129}I, ^{81}Kr and Sb. For most contaminants (such as ^{39}Ar), the amounts remaining in the vault, geosphere and biosphere are less than the initial inventory because of radioactive decay. A few others (such as ^{231}Pa) show larger amounts because of ingrowth from their precursors.

** A "Z" after the symbol for an element or radionuclide indicates it is from the Zircaloy waste matrix. All other contaminants are from the used-fuel (UO_2) waste matrix.
The nine chemically toxic elements are bromine (Br), cadmium (Cd), chromium (Cr), molybdenum (Mo), antimony (Sb), selenium (Se), samarium (Sm) and technetium (Tc).
The postclosure assessment examines a total of 68 distinct radionuclides (Section 5.9). However, 13 radionuclides are evaluated twice because they are found both in used fuel and in Zircaloy. Of these 81 (68+13) radionuclides, only 57 are listed here. The other 24 are not directly simulated in the vault and geosphere models, but they are approximated in the biosphere using arguments based on secular equilibrium. Our results show that for times up to 10^5 a, these 24 radionuclides would have no significant discharges to the biosphere. The 24 radionuclides not listed are:
^{225}Ac ^{227}Ac ^{210}Bi ^{93m}Nb ^{93m}Nb Z ^{32}P ^{32}P Z ^{233}Pa
^{210}Pb ^{210}Po ^{223}Pa ^{224}Ra ^{225}Ra ^{228}Ra ^{222}Rn ^{126}Sb
^{182}Ta ^{125m}Te ^{125m}Te Z ^{227}Th ^{228}Th ^{231}Th ^{234}Th and ^{90}Y.

natural barriers in restricting and delaying the movement of contaminants to the biosphere.

Figure 6-5 shows the distribution of ^{129}I, the contaminant with the greatest contribution to radiation dose, after periods of 10^4 a and 10^5 a following closure. The initial inventory of ^{129}I in the used-fuel matrix amounts to 56 100 mol (or 7240 kg). Part (a) of the figure indicates that, at 10^4 a, most of the initial inventory of ^{129}I remains in the containers and waste matrices; only about 3.9% has been transported to the buffer and backfill, and no significant quantity (less than 10^{-15} mol) has reached the biosphere. Part (b) of the figure gives the status after 10^5 a: about 93% of the initial inventory of ^{129}I still remains in the containers and waste matrices; 5.5% is in the buffer and backfill, and 0.9% has entered the geosphere. Only 0.0005% has entered the biosphere. The estimated maximum rate entry of ^{129}I into the biosphere, for times up to 10^5 a, is about 3×10^{-6} mol/a to well water and 9×10^{-6} mol/a into the discharge zone in Boggy Creek South.

Figure 6-6 gives the distribution of ^{14}C at 10^4 a and at 10^5 a following closure. The initial inventory of ^{14}C in the used-fuel matrix is 2980 mol (or 41.7 kg). After 10^5 a, most of this initial inventory has decayed before it can leave the containers and waste matrices. Only minute amounts have reached the geosphere (about 1.8 mol), where further decay is significant. Extremely small amounts reach the biosphere. The estimated maximum rates of entry of ^{14}C to the biosphere are about 1×10^{-11} mol/a to well water and 2×10^{-12} mol/a into the discharge zone in Boggy Creek South.

Figure 6-7 indicates the distribution of ^{99}Tc after 10^4 a and 10^5 a following closure. The initial inventory of ^{99}Tc in the used-fuel matrix is 335 000 mol (or 33 200 kg), and the effects of radioactive decay are important (although less so than for ^{14}C). The effect of chemical precipitation in the buffer and sorption in the buffer and backfill can be inferred by comparing the relative quantities of ^{99}Tc that enter and exit the buffer and backfill. In 10^5 a, 2×10^{-10} mol have been released to the geosphere, but no significant quantity has entered the biosphere.

Figure 6-8 illustrates the distribution of ^{238}U after 10^4 a and 10^5 a following closure. This is the most abundant isotope in the used-fuel matrix, with an initial inventory of 6.70×10^8 mol (or 1.59×10^8 kg). Most of this contaminant is retained in the UO_2 waste matrix. In 10^5 a, only 1.2×10^{-11} mol have been released to the geosphere, with none entering the biosphere.

Of the nine chemically toxic contaminants, bromine has the largest estimated release to the biosphere, amounting to 2.4×10^{-2} mol by 10^5 a, with a maximum release rate of less than 1.2×10^{-6} mol/a. Estimated releases for the other eight chemically toxic contaminants (antimony, cadmium, cesium, chromium, molybdenum, samarium, selenium and technetium) are 9 or more orders of magnitude smaller. The resulting estimated concentrations in the biosphere are very small; for example, we obtain a value of less than 3×10^{-10} mol of bromine per kg of soil. This value is more than 5 orders of magnitude smaller than median concentrations of bromine in the environment (Bowen 1979). At these very small concentrations, bromine (and the other chemically toxic contaminants) would have negligible chemical toxicity impacts.

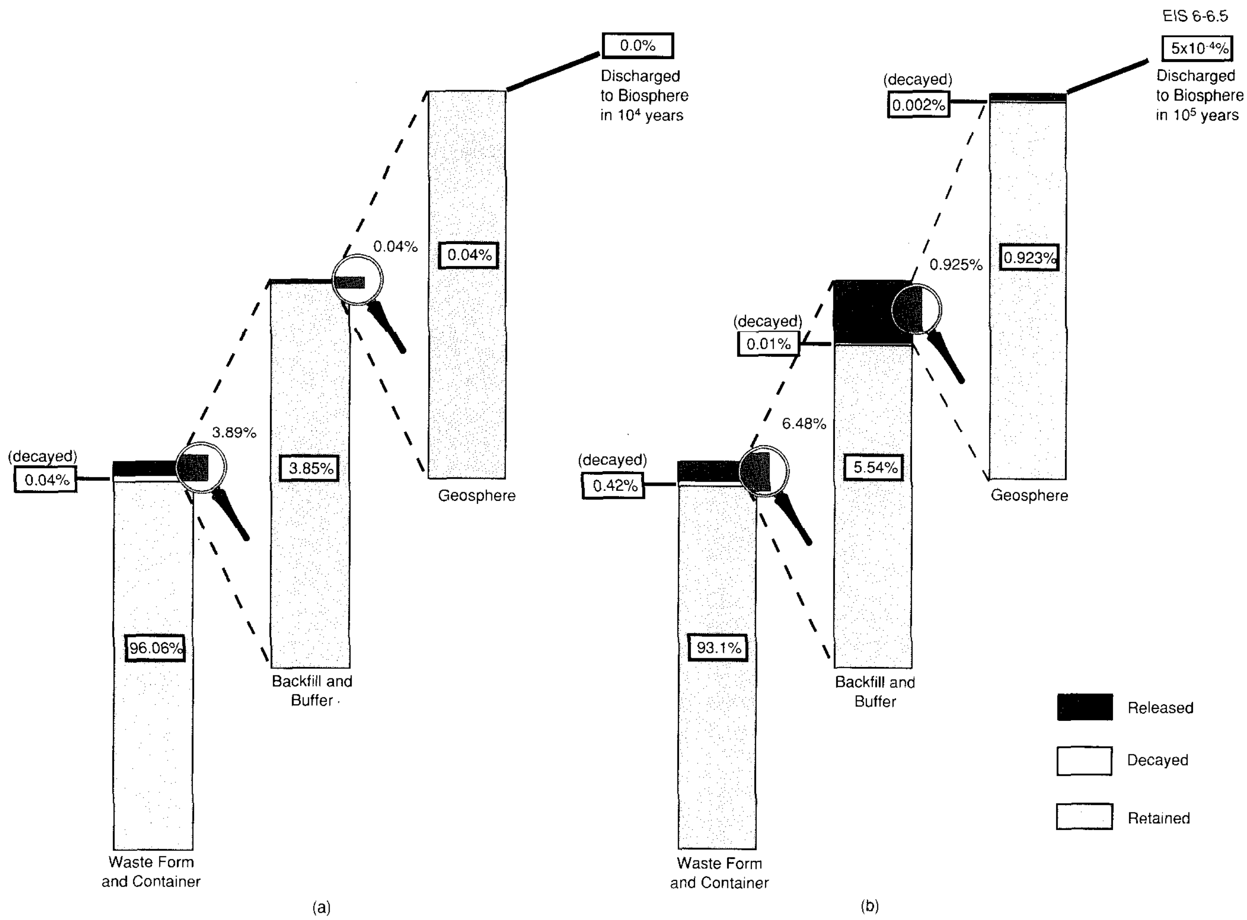

FIGURE 6-5: Distribution of ^{129}I in the Disposal System for the Median-Value Simulation

Parts (a) and (b) show the predicted distributions after 10^4 and 10^5 a respectively. All percentage values are expressed relative to the initial inventory of ^{129}I (56 100 mol). Most of the ^{129}I is retained in the vault containers and used-fuel matrix, and successively smaller percentages are found in the vault buffer and backfill and in the rock of the geosphere. Essentially no ^{129}I is released to the biosphere for times up to 10^4 a, and only small quantities are released for times up to 10^5 a. For times up to 10^5 a, all the discharges are predicted to occur at Boggy Creek South and to the well, with no discharges to Boggy Creek North or Pinawa Channel.

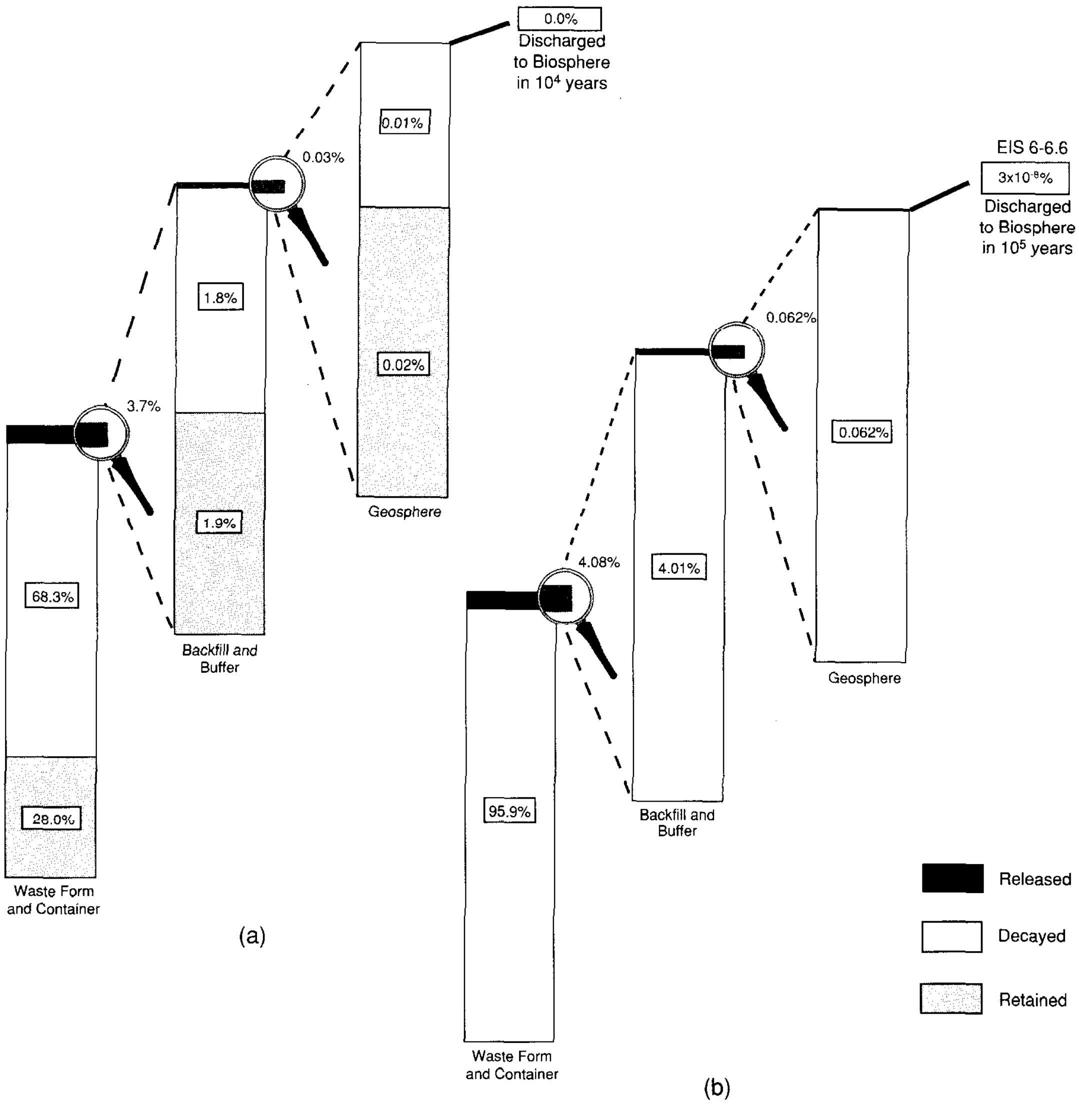

FIGURE 6-6: Distribution of ^{14}C from Used Fuel in the Disposal System for the Median-Value Simulation

Parts (a) and (b) show the predicted distributions after 10^4 and 10^5 a respectively, from the ^{14}C in the used-fuel waste matrix. All percentage values are expressed relative to the initial inventory of ^{14}C (2980 mol). Radioactive decay is significant in reducing ^{14}C inventories in different sections of the system because ^{14}C has a relatively short half-life (5730 a). Most of the ^{14}C remains or decays in the vault containers and in the used-fuel matrix. Successively smaller percentages remain in the vault buffer and backfill and the rock of the geosphere. At 10^5 a, a very small amount of ^{14}C has discharged to Boggy Creek South and to the well. There are no discharges of ^{14}C to Boggy Creek North or Pinawa Channel, even after 10^5 a.

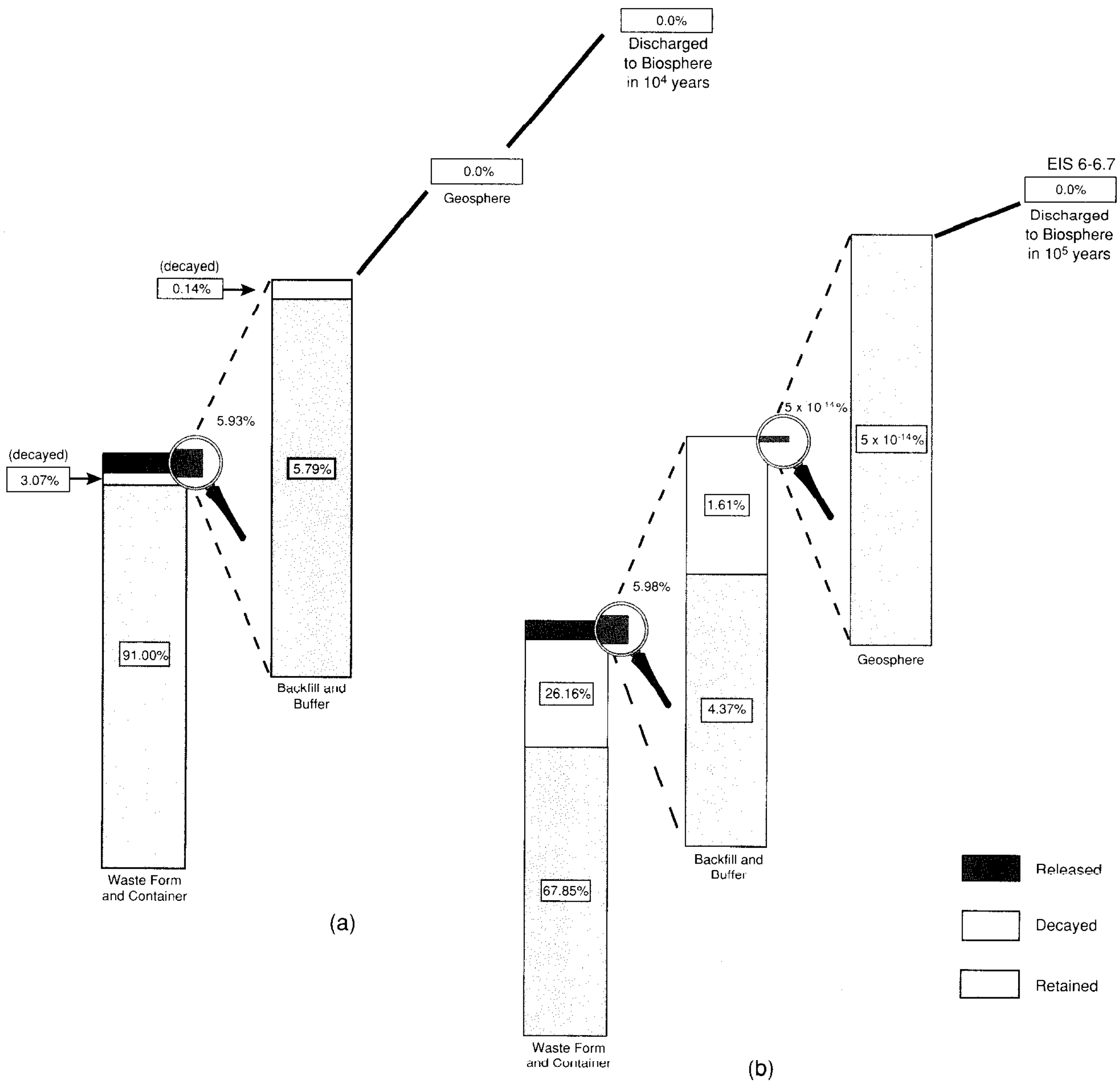

FIGURE 6-7: Distribution of ^{99}Tc in the Disposal System for the Median-Value Simulation

Parts (a) and (b) show the predicted distributions after 10^4 and 10^5 a respectively. All percentage values are expressed relative to the initial inventory of ^{99}Tc (335 000 mol). Radioactive decay is important in reducing ^{99}Tc inventories in different sections of the disposal system. Most of the ^{99}Tc is retained in the vault containers and in the used-fuel matrix. Successively smaller percentages are found in the vault buffer and backfill and in the rock of the geosphere. There are no significant discharges of ^{99}Tc to the biosphere, even after 10^5 a.

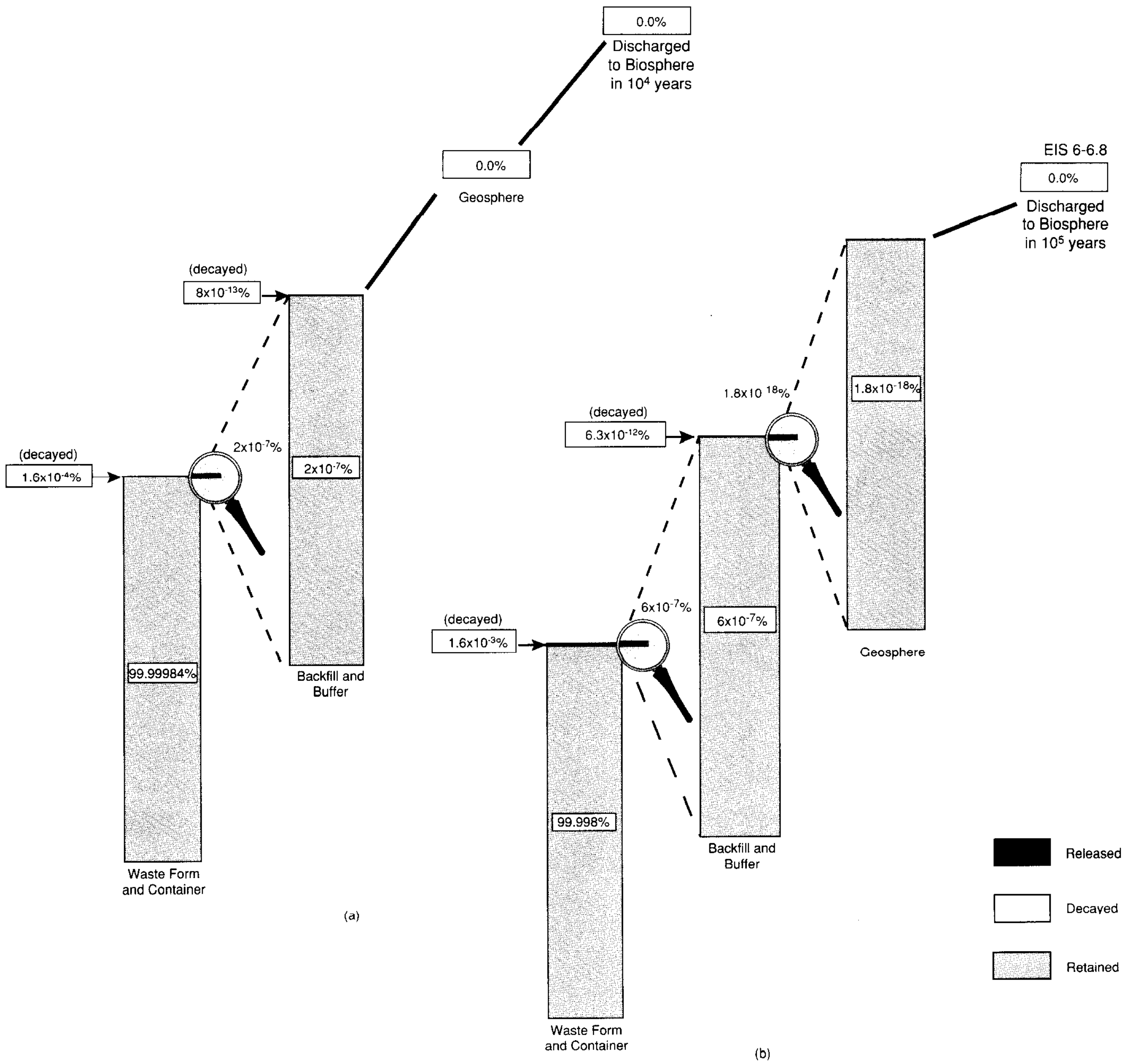

FIGURE 6-8: Distribution of ^{238}U in the Disposal System for the Median-Value Simulation

Parts (a) and (b) show the predicted distributions after 10^4 and 10^5 a respectively. All percentage values are expressed relative to the initial inventory of ^{238}U (6.7×10^8 mol), the most abundant isotope in the used-fuel matrix. Most of the ^{238}U is retained in the vault containers and in the used-fuel matrix. Successively smaller percentages are found in the vault buffer and backfill and in the rock of the geosphere. There are no significant discharges of ^{238}U to the biosphere, even after 10^5 a.

Calculations for the median-value simulation also involve estimates of dose rate to four generic target organisms (Section 5.6.2.8): a plant, a mammal, a bird and a fish. Their characteristics, habitat and resource utilization are expected to represent a wide range of organisms. The results show that the largest estimated dose rates are due to ^{129}I and ^{14}C:

- The estimated dose rate to the plant is 9 x 10^{-9} Gy/a from ^{14}C and 1 x 10^{-6} Gy/a from ^{129}I. (The gray differs from the human unit of dose, sievert, by a dimensionless quality factor, which has a value of unity for ^{14}C and ^{129}I). Over 98% of the estimated dose rate is due to leaf uptake from irrigation.

- The estimated dose rate to the mammal is 2 x 10^{-8} Gy/a from ^{14}C and 3 x 10^{-6} Gy/a from ^{129}I. Over 90% of the estimated dose rate is due to ingestion of well water.

- The estimated dose rate to the bird is 2 x 10^{-8} Gy/a from ^{14}C and 1 x 10^{-5} Gy/a from ^{129}I. Over 93% of the estimated dose rate is due to ingestion of well water.

- The estimated dose rate to the fish is 2 x 10^{-8} Gy/a from ^{14}C and 7 x 10^{-8} Gy/a from ^{129}I. Over 95% of the estimated dose rate is internal, caused by ingestion of contaminated food and surface water.

These dose rates generally are much smaller than the range of dose rates to plants and animals from natural sources; for example, total dose rate from natural, external sources is typically about 7 x 10^{-4} Gy/a in Canada (Health and Welfare Canada 1986).

6.3.3 Sensitivity Analysis of the Median-Value Simulation

6.3.3.1 The Method Used for Sensitivity Analysis

Sensitivity analysis of the median-value simulation extends our understanding of the workings of the system model: it shows how selected output of the model changes with variations in parameters and other features of the model. Sensitivity analysis of the median-value simulation also contributes to the interpretation of the probabilistic results (discussed in Section 6.5).

Sensitivity analyses involving the use of median values are described in several places.

- Section 6.2 describes results aimed at the development of derived constraints and pertains only to selected design parameters.

- Section 6.3.2 (and Sections D.2 to D.4 in Appendix D) describes the analysis of the median-value simulation and includes discussion of the sensitivity of results to important processes, pathways and radionuclides.

- Section 6.4 documents a special study of barrier effectiveness.

In the following discussion, we summarize the systematic sensitivity analyses performed for the median-value simulation and aimed at identifying the "important" parameters from among all the parameters in the system model. An important parameter is defined as one that causes a notable change to an objective function when the value of the parameter is changed.

The objective functions of most interest are the maxima up to 10^5 a of the total ADE to an individual in the critical group from all radionuclides and the ADEs from ^{14}C alone and from ^{129}I alone. Section D.5 in Appendix D discusses why these particular objective functions were chosen and gives examples of several others. (Other objective functions examine the performance of the vault, geosphere and biosphere, and are documented in Sections D.6 to D.8 in Appendix D.) Section D.5 in Appendix D also details the method used for these sensitivity analyses: the major tool used to screen for important parameters is iterated fractional factorial analysis (described in Section A.4 in Appendix A).

Once a parameter has been identified as important, we proceed with investigations to show how and why it influences the results. Sections D.6 to D.8 in Appendix D document these investigations for results from the vault, geosphere and biosphere models.

Other sensitivity analyses are documented in the primary references for the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993). Results in these documents generally agree with the results presented here; any differences can be attributed to the differences in the models or objective functions used in the analyses. The studies reported in this document all refer to the system model representing the entire reference disposal system, whereas the results and the studies described in the primary references for the vault, geosphere and biosphere models frequently pertain to only part of the system model.

In performing the sensitivity analysis, we examine three general classes of input parameters. The first class contains sampled parameters whose values are uncertain; they are described using PDFs with a continuous range of feasible values (Figure A-6 in Appendix A gives examples of PDFs). Two other classes of parameters are switches and constants:

- Switches select one option from a group of mutually exclusive options for a simulation. For example, there is a switch in the biosphere model that describes the source of the domestic water used by the critical group: it may be either the well or the lake. Changing the value of a switch changes the option selected and may induce large changes in the ADE. Switches are described using piecewise uniform PDFs (Figure A-6 in Appendix A) defined so that each possible option is sampled according to its prescribed probability of occurrence.

- Constants are used for parameters that are considered to have a single well-defined value. The effective thickness of the container walls, for example, is fixed at 4.2 mm because it is a controlled design parameter. Nevertheless, it is of interest to understand how changes in some constant parameters, such as effective thickness of the container walls, would affect estimated dose or performance measures. Thus sensitivity analysis includes the study of variations of constant parameters of interest (provided that such variations do not lead to major inconsistencies in the model). Results for some of the 788 constant parameters that were examined are reported in Section 6.3.3.5. Section 6.2 describes results for some constant parameters of interest for the development of derived constraints. (Section 6.6 also examines the effects of changing some constant parameters in a study of selected design and site features, using sets of randomly sampled simulations.)

6.3.3.2 Effects of Small Variations of Important Parameters

Table 6-2 summarizes the results of the screening process for small variations of parameters about their median values. The process is equivalent to a conventional sensitivity analysis that determines a partial derivative of an output variable with respect to a single input parameter.

The parameters considered are those that are described using PDFs in the probabilistic analysis. The table lists the parameters that have the greatest effect on the maximum ADE from ^{14}C and ^{129}I when varied near their median values and with all other parameters fixed at their median values.

Definitions for some of the less familiar parameters in Table 6-2 are provided below.

- Tortuosity in rock is a measure of the effective increased transport distance for diffusion because of the winding nature of the interconnected aqueous pathway within the rock (Davison et al. 1994b).

- The plant/soil concentration ratio for an element describes the relationship between concentrations of the element in plants and in the soil on which they grow (Davis et al. 1993).

- The gaseous evasion rate from soil for an element is the rate constant describing the loss of the (volatile) element from soil by degassing (Davis et al. 1993).

- The instant-release fraction for ^{14}C describes the fraction of ^{14}C in used fuel released by the instant-release mechanism (Johnson et al. 1994b; Section 5.2.2).

- The buffer anion correlation parameter correlates values of the diffusion coefficient and capacity factors in the buffer for anionic species (Johnson et al. 1994b; Section 5.7).

- The groundwater velocity scaling factor is a dimensionless multiplicative factor used to describe the uncertainty in groundwater velocities in the geosphere (Davison et al. 1994b).

TABLE 6-2

EFFECTS OF SMALL VARIATIONS OF IMPORTANT PARAMETERS ON ESTIMATED ANNUAL DOSE TO 10^5 a

Important Parameter*	Percentage Difference* in Maximum ADE for Times up to 10^5a from	
	^{129}I	^{14}C
Tortuosity of the lower rock zone	-30	-50
Plant/soil concentration ratio for iodine**	-30	0.0
Gaseous evasion rate from soil for iodine	-11	0.0
Free-water diffusion coefficient for iodine	6.8	0.0
Buffer anion correlation parameter	6.2	8.6
Groundwater velocity scaling factor	-5.7	3.7
Initial inventory of ^{129}I in used fuel	5.1	0.0
Initial inventory of ^{14}C in used fuel	0.0	23
Free-water diffusion coefficient for carbon	0.0	11
Instant-release fraction for ^{14}C	0.0	9.2
Gaseous evasion rate for carbon from soil	0.0	-9.1
Plant/soil concentration ratio for carbon	0.0	8.6

* The parameters listed are those identified as important for small variations in values near the median value. That is, they have the greatest effect on the maximum ADE from ^{14}C or ^{129}I for times up to 10^5 a when their values are changed from their 0.475 to 0.525 quantile values. The percentage differences are calculated from the formula:

$$100 \times \frac{\text{Max ADE (.525 quantile) - Max ADE (.475 quantile)}}{\text{Max ADE (0.500 quantile)}}$$

where Max ADE (Q quantile) is the maximum ADE up to 10^5 a when the indicated parameter value corresponds to its Q quantile, and all other parameters are fixed at their median value (which is the 0.500 quantile). A difference of 0.0% implies no effect. A negative value implies a negative correlation, as is the case for tortuosity of the lower rock zone (increasing the tortuosity leads to decreased ADEs).

** The negative value suggests that ADEs are negatively correlated with the plant/soil concentration ratio for iodine. However the discussion in Section D.8.3 in Appendix D states the opposite (see Figure D-62); that is, larger ADEs are associated with larger concentration ratios. The discrepancy arises because the soil model uses two different algorithms, and their domains change near the value corresponding to the 0.5 quantile. Because the two algorithms are somewhat discontinuous, a negative value (-30) is calculated for this table. Thus the value reported here is mathematically correct, but it is an artifact of the soil model. Annual dose estimates are actually positively correlated with the plant/soil concentration ratio when considering the larger range of feasible values.

As indicated in the table, tortuosity of the lower rock zone is the most important parameter: its variation around the median value results in the greatest changes to the maximum ADEs from ^{14}C and ^{129}I. Larger tortuosities correspond to longer diffusive flow paths, and the resultant delays in contaminant transport yield smaller ADEs. Its effect is more pronounced for ^{14}C than for ^{129}I because ^{14}C has a much shorter half-life, so that less ^{14}C survives to reach the biosphere (Sections D.6 and D.7 in Appendix D). Table 6-2 also shows that

- Four parameters have large effects on the maximum ADE resulting from ^{129}I only: the plant/soil concentration ratio for iodine, the gaseous evasion rate from soil for iodine, the free-water diffusion coefficient for iodine, and the initial inventory of ^{129}I in used fuel.

- Five others affect the ADEs from ^{14}C only. They are the initial inventory of ^{14}C in used fuel, the free-water diffusion coefficient for carbon, the instant-release fraction for ^{14}C, the gaseous evasion rate from soil of carbon, and the plant/soil concentration ratio for carbon.

- In general, parameters used to characterize one nuclide do not affect doses from other nuclides; thus the percentage difference is zero for the ADEs from ^{14}C when the initial inventory of ^{129}I is changed.

- Two remaining parameters affect the maximum ADE resulting from ^{129}I and ^{14}C: the buffer anion correlation parameter and the groundwater velocity scaling parameter. One unusual result shows that an increase in the groundwater velocity scaling factor leads to an increase in the maximum ADE resulting from ^{14}C but a decrease from ^{129}I, a consequence of the competing influences of radioactive decay, groundwater dilution and radionuclide travel time on the estimated amount of a radionuclide that discharges to the biosphere.

The results in Table 6-2 show separately the effects on radiation doses from ^{14}C and from ^{129}I. A consideration of effects on the total radiation doses from both radionuclides shows results identical to the results for ^{129}I alone, because ^{129}I dominates the ADEs (Figure 6-4). Put another way, variations in a parameter such as the initial inventory of ^{14}C would show little effect on the total radiation dose.

For some parameters, it is possible to observe subtle effects relating to parameter uncertainty. One such case occurs because of the uncertainty (or range of possible values) in the initial inventories of ^{14}C and ^{129}I in used fuel. Table 6-2 shows that using the 0.475 and 0.525 quantiles of initial inventory leads to a 23% change in the maximum ADE from ^{14}C but only a 5.1% change for ^{129}I. From the functional relationship specified in the system model, the ADE from any radionuclide should be directly proportional to its inventory (possible complicating effects, such as chemical precipitation and isotopic dilution are not important here). The differential effects of the two nuclides can be attributed to the differences in the uncertainties of their initial inventories. As might be expected from the results in Table 6-2, the inventory data show that ^{14}C has a wider range of uncertainty than ^{129}I. In fact, the differences in inventory in used fuel between the 0.475 and 0.525 quantiles correspond exactly to 23% for ^{14}C and 5.1% for ^{129}I.

Sections D.6 to D.8 in Appendix D provide further insight into how the above parameters affect the results and why they are important.

6.3.3.3 Effects of Full-Range Variation of Important Parameters

Section 6.3.3.2 is concerned with parameters that are important in a small range of values near the median values. In this section, we expand the analysis to examine what happens when considering the entire range of possible values of each parameter. For this median-value sensitivity analysis, only the one parameter at a time is allowed to vary, over its full range, while all other parameters are fixed at their median values. For the probabilistic sensitivity analysis (Section 6.5.5), we also use the entire range of possible values for each parameter, but all parameters are allowed to vary at the same time.

Table 6-3 summarizes the results of the screening process in which parameter variations cover their entire range of possible values. The results in Table 6-3 are somewhat different from Table 6-2 because the relative importance of some parameters depends on whether we examine small variations about the median value or the full range of possible values.

Table 6-3 shows how changes in each important parameter affect the maximum ADEs (up to 10^5 a) that result from ^{14}C and ^{129}I. The data in the table show ratios of the largest to smallest of the maximum ADEs that were observed in simulations in which the important parameters are individually given values corresponding to specified quantiles, with all other parameters fixed at their median values. The results show that

- The tortuosity of the lower rock zone has the largest ratios for ^{14}C and ^{129}I. Tortuosity has a much greater effect on ADEs resulting from ^{14}C than from ^{129}I because of the the smaller half-life of ^{14}C. The other parameters have somewhat lesser effects on these ratios.

- Four other parameters affect the ratios for both nuclides: the depth of the well, the buffer anion correlation parameter, the groundwater velocity scaling factor, and the number of persons in the critical group. Three of these parameters affect both the ^{14}C and ^{129}I ratios by approximately the same amount (within a multiplicative factor of 3), whereas the fourth (the groundwater velocity scaling factor) affects the ratio for ^{14}C much more strongly than the ratio for ^{129}I. The main reason for this differential effect is because of the relatively short half-life of ^{14}C compared with that of ^{129}I (Section D.7.3 in Appendix D).

TABLE 6-3

EFFECTS OF FULL-RANGE VARIATIONS OF IMPORTANT PARAMETERS ON ESTIMATED ANNUAL DOSE TO 10^5 a

Important Parameter*	Ratio** of the Largest to the Smallest Maximum ADE up to 10^5 a Resulting from ^{129}I	^{14}C
Tortuosity of the lower rock zone	3600	360 000
Depth of the well***	100	270
Free-water diffusion coefficient for iodine	73	1
Initial inventory of ^{129}I in used fuel	32	1
Buffer anion correlation parameter	25	43
Instant-release fraction for ^{129}I	18	1
Groundwater velocity scaling factor	6	13 000
Aquatic mass loading coefficient for iodine	4	1
Iodine plant environmental half-life	3	1
Number of persons per household	3	3
Initial inventory of ^{14}C in used fuel	1	100
Free-water diffusion coefficient for carbon	1	690
Instant-release fraction for ^{14}C	1	25

* The parameters listed are those identified as important for large variations in their values: they have the greatest effect on the maximum annual dose estimate (ADE), for times up to 10^5 a, when their values are changed over their full range of acceptable values. (For most parameters, the values examined correspond to the following quantiles: 0.0, 0.02, 0.05, 0.1, 0.2, 0.3, 0.4, 0.51, 0.6, 0.7, 0.8, 0.9, 0.95, 0.98 and 1.0. For some parameters, the 0.0 and 1.0 quantiles were excluded because their PDFs are either unbounded (as for "aquatic mass loading coefficient for iodine") or are very broad. For "number of persons per household" (of the critical group), values used ranged from 1 to 36.)

** The data show the ratios of the largest to smallest maximum ADEs that are observed when each parameter is varied separately over its range and when all other parameters are fixed at their median values. A ratio equal to unity implies no effect.

*** The importance of depth of the well is partly an artifact of the full-range variations (see text).

- Five parameters have large effects only for ^{129}I: the free-water diffusion coefficient for iodine, the initial inventory in used fuel of ^{129}I, the instant-release fraction of ^{129}I, the aquatic mass loading coefficient (from the lake) for iodine (describing the degassing of iodine from surface water) and the iodine plant environmental half-life (or residence time of iodine deposited on plants).

- Three parameters have large effects only for ^{14}C: the initial inventory of ^{14}C in used fuel, the free-water diffusion coefficient of carbon and the instant-release fraction of ^{14}C.

- As in the analysis of small variations, parameters used to describe characteristics of one nuclide have no effect on the estimated doses produced by another nuclide, and thus the ratio for ^{14}C is unity (that is, there is no difference) when the initial inventory of ^{129}I is changed.

- Some parameters identified as important for small-range variations (Table 6-2) are not important for large-range variations. These parameters are the plant/soil concentration ratios and the gaseous evasion rates from soil for carbon and for iodine.

- In contrast, five additional parameters are important only for large-range variations: depth of the well, instant-release fraction for ^{129}I, aquatic mass loading coefficient for iodine, iodine plant environmental half-life, and number of persons in the critical group.

  Further analysis shows that the importance of the depth of the well is partly an artifact of the sampling procedure, and it is not as important as Table 6-3 suggests. In the full-range variation of values for this parameter, large values correspond to the selection of a bedrock well that intercepts the contaminant plume moving up LD1. However, small values correspond to selection of an overburden well, and contaminant concentrations in an overburden well are set equal to contaminant concentrations in the lake (Section 5.5). Thus the importance of the using small or large depths of the well in the full-range analysis is similar to the use of the lake or a bedrock well as the source of domestic water. (We show in the next section that the switch parameter that selects the source of domestic water is an important parameter.) If our full-range analysis were restricted to bedrock wells only or to overburden wells only, the depth of the well would be less important. This last result is discussed further in Section D.7.4 of Appendix D.

As before, results obtained for the maximum ADE from both nuclides are identical to the results for ^{129}I alone, because ^{129}I dominates the maximum ADE (Figure 6-4). Sections D.6 to D.8 in Appendix D provide further discussion on the underlying reasons for these effects, including the reasons for differences between Tables 6-2 and 6-3.

6.3.3.4 Effects of Changing Switch Values

All switches in the system model were varied one at a time, examining each possible value, when all other parameters and switches were fixed at their median-case values. For most switch parameters in SYVAC3-CC3, the median value also corresponds to the most probable value; this is the case for irrigation of the garden, soil type and fresh lake sediment used as soil (see Table 6-4). For the switch selecting the source of domestic water, the probabilities of occurrence are 0.50 for both the lake and the well (Davis et al. 1993). We have defined the well to be the source of domestic water in the median-value simulation.

Four of the switches in the system model have a significant influence on the maximum ADE from ^{14}C or ^{129}I up to 10^5 a after closure; their effects are summarized in Table 6-4. The important switches are

- Source of domestic water, describing the choice between the use of lake water or well water as the source of domestic water used by the critical group.

- Irrigation of the garden, which determines whether a simulation does or does not include irrigation of the garden. The source of water for irrigation is the same as the domestic water supply unless the tentative well demand exceeds well capacity, in which case we assume that the lake supplies irrigation water (Sections 5.5 and 5.6).

- Soil type, which allows the selection of four different types of soil in the garden, forage field and wood lot.

- Lake sediment as soil, allowing the possible use of fresh lake sediment to replace or augment the soil in the garden, forage field, wood lot and peat bog.

Other switches, such as the one that selects the source of heating fuel used by the critical group (wood or peat), are not identified as important.

The results in Table 6-4 show that

- The switch selecting the source of domestic water has the largest effects. The maximum ADEs resulting from ^{14}C and ^{129}I are about 2 orders of magnitude larger if the source of water is the well instead of the lake.

- The switches selecting soil type and whether the garden is irrigated have smaller effects. For both nuclides, the maximum ADEs are larger for organic soil and for simulations in which the garden is irrigated.

- The switch selecting fresh lake sediment used as soil has a relatively large effect for ^{14}C but little effect for ^{129}I.

An overall implication is the effects of these switches on the total ADEs from both ^{129}I and ^{14}C would be similar to the effects on ^{129}I only, because the ADEs from ^{129}I are more than 200 times greater than the ADEs from ^{14}C in all cases. Thus larger radiation doses would occur when the well is the source of domestic water, the soil type is organic or the garden is irrigated. Smaller doses would occur when fresh lake sediment is used as soil.

The reasons underlying these effects are included with the detailed discussion of sensitivity-analysis results from the biosphere model (Section D.8 in Appendix D).

TABLE 6-4

EFFECTS OF CHANGES IN IMPORTANT SWITCHES ON ESTIMATED ANNUAL DOSE TO 10^5 a

Switch Description*	Options Available and Probability of Occurrence**		Effect of Using the Option on the Ratio of Maximum ADE*** ^{129}I	^{14}C
Source of Domestic Water	Well**	(0.50)	1.0	1.0
	Lake	(0.50)	0.01	0.005
Irrigation of Garden	Yes**	(0.90)	1.0	1.0
	No	(0.10)	0.32	0.34
Soil Type	Sand**	(0.57)	1.0	1.0
	Loam	(0.05)	1.6	1.2
	Clay	(0.24)	1.6	1.5
	Organic	(0.14)	2.7	8.6
Fresh Lake Sediment Used as Soil	Yes	(0.01)	0.9	50.0
	No**	(0.99)	1.0	1.0

* The four switches listed are those identified as important for the median-value simulation. That is, each indicated switch has a significant effect on the maximum annual dose estimate (ADE) resulting from ^{14}C or from ^{129}I for times up to 10^5 a, when it selects different options and when all other parameters (including all other switches) are fixed at their median values.

** The probability of occurrence for different options is taken from the PDF used to characterize the switch in the probabilistic analysis. The option flagged is that chosen for use in the median-value simulation.

*** The data in the last two columns show the effects of the switches for the different options. The effects reported are ratios of maximum ADEs: the estimate obtained using the indicated option divided by the estimate obtained from the median-value simulation. A ratio of unity indicates two possibilities: the specified option has no effect or the specified option is identical to that used in the median-value simulation.

6.3.3.5 Effects of Varying Constant Parameters

The changes to the constant parameters are considered individually. After varying a total of 788 parameters that are normally fixed in value, we observed that only a few have large effects on the maximum ADE up to 10^5 a.

An important observation from these studies is that the ADEs resulting from ^{14}C and ^{129}I are sensitive to the closest distance between the waste emplacement part of a vault room and fracture zone LD1 (the waste exclusion distance), decreasing in magnitude as the distance is increased. Figures 6-9 and 6-10 show results from six simulations that correspond to moving

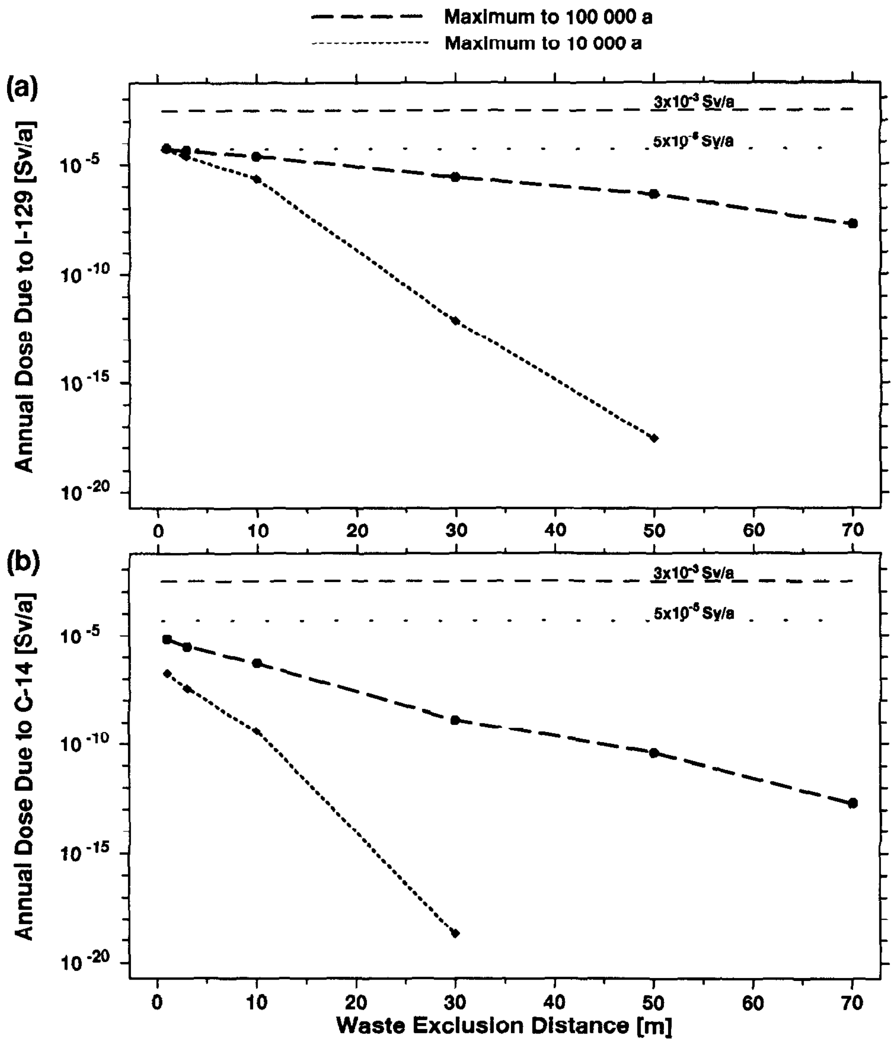

FIGURE 6-9: Effect of the Waste Exclusion Distance

The waste exclusion distance is the length of sparsely fractured rock between fracture zone LD1 and the waste emplacement part of the nearest vault room. Results shown are from six simulations in which the distance is about 1, 3, 10, 30, 50 and 70 m. Parts (a) and (b) show the maximum, for times up to 10^4 a and up to 10^5 a, ADEs from ^{129}I and ^{14}C. The two horizontal lines show the annual dose associated with the AECB *risk criterion* (5 x 10^{-5} Sv/a) and a typical annual dose from radiation in the natural environment (3 x 10^{-3} Sv/a).
The curves show that the ADEs are strongly influenced by the length of the waste exclusion distance, especially at 10^4 a. However, even small lengths of rock are effective in delaying and attenuating estimated annual doses.

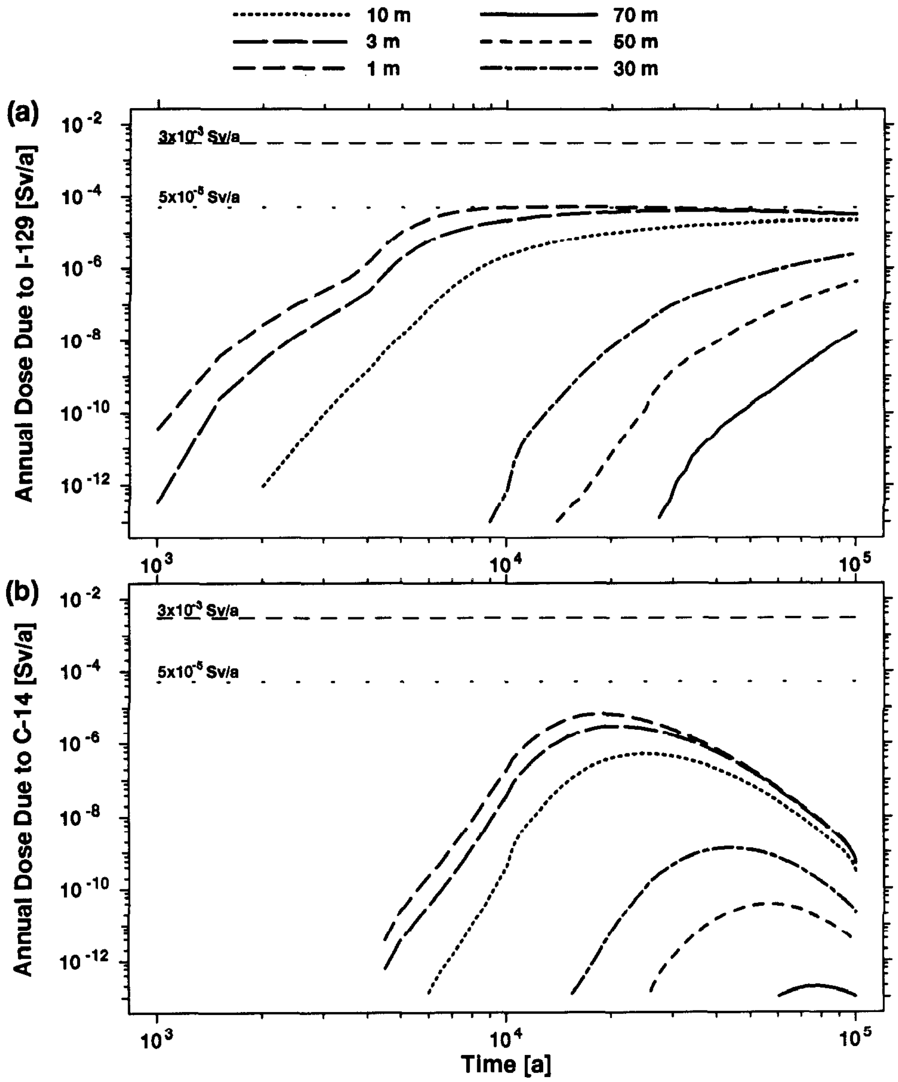

FIGURE 6-10: Dose-Time Curves for Different Waste Exclusion Distances

The waste exclusion distance is the length of sparsely fractured rock between fracture zone LD1 and the waste emplacement part of the nearest vault room. Other comments are as for Figure 6-9, except that the horizontal axes show the time.
The curves show that longer waste exclusion distances are more effective in attenuating and delaying estimates of annual dose, with greater attenuation for short-lived ^{14}C than for long-lived ^{129}I.

the vault toward or away from LD1 (in a horizontal plane) to achieve waste exclusion distances ranging from about 1 m to about 70 m. Each simulation uses different Cartesian coordinates and hydraulic heads for the network nodes (adjusted to conform with the detailed results from MOTIF, as described in Section 5.4). All other parameters have been fixed at their median values. The figures show that

- The length of the waste exclusion distance has a strong influence on the maximum ADEs to 10^4 a and a weaker effect at 10^5 a (Figure 6-9). The effects are more significant at early times where the dose-time curves are rising faster (Figure 6-10). Even when there is only about 1 m of sparsely fractured rock between LD1 and the nearest containers in the vault, ADEs for ^{129}I are less than the total annual dose from natural background and just slightly above the annual dose associated with the AECB risk criterion (5 x 10^{-5} Sv/a).

- The time of occurrence of the maximum value of the ADEs moves to later times for longer waste exclusion distances. The effect is best shown for ^{14}C in part (b) of Figure 6-10; it shows maxima for all waste exclusion distances studied because of the interactions between transport time and half-life. There is a large decrease in the magnitudes of the maxima from ^{14}C because longer waste exclusion distances mean less ^{14}C survives the radioactive decay and is available for discharge into the biosphere.

  The time of occurrence of the maximum ADE from ^{129}I also moves to later times for longer distances: the maximum occurs before 10^4 a with a distance of 1 m, between 10^4 and 10^5 a with a distance of 3 m, and at 10^5 a (the time cutoff of the simulations) with distances of 10, 30, 50 and 70 m. Because ^{129}I has a longer half-life, the magnitudes of its maxima are not as strongly affected (compared with ^{14}C). With a 1-m distance, the maximum for ^{129}I occurs before the maximum for ^{14}C because of the retardation (sorption) of ^{14}C onto minerals in fracture zone LD1 and in the upper rock zone (see Table D-2).

- The two figures show that the waste exclusion distance is effective in attenuating and delaying impacts, with the greater attenuation for short-lived ^{14}C.

Sections 6.2 and 6.6 provide further discussion on the effects of the length of the waste exclusion distance.

Other general observations on the sensitivities of the constant parameters are as follows:

- The maximum ADEs resulting from ^{14}C increase if the radioactive half-life of ^{14}C is increased, whereas the opposite effect occurs if the half-life of ^{129}I is increased. (Radionuclide half-lives are generally well known, but we have examined simulations with different values to help reveal and understand interactions in the system model.) This observation can be attributed to two competing factors related to radioactive decay: inventory and activity. In the system model, the estimated dose resulting from a radionuclide is proportional to its inventory reaching the biosphere and to its specific activity (related to the number of disintegrations per unit time and per unit mass). The inventory factor increases with increasing half-life because a greater fraction of the initial radionuclide inventory will survive the transport from the waste matrix to the biosphere. In contrast, the specific activity factor is inversely proportional to half-life; that is, long-lived radionuclides are less radioactive per unit time than short-lived radionuclides.

For parameter values in the median-value simulation, slightly greater values for the long half-life of ^{129}I (1.6 x 10^7 a) lead to smaller estimates of dose because of the reduced specific activity; there is little change (in 10^5 a) in the amount of ^{129}I that survives. Conversely, slightly greater values for the half-life of ^{14}C (5.7 x 10^3 a) lead to greater estimates of dose, because the effects of reduced specific activity are outweighed by the increased inventory of ^{14}C that survives transport.

- Estimates of releases from the vault and annual dose increase with increasing amounts of used fuel in the vault. The reason is clear: increasing the mass of used fuel also increases the initial inventories of all contaminants, which leads to proportional increases in estimated releases from the vault and geosphere, and increased estimates of annual doses.

- The ADEs resulting from ^{14}C and ^{129}I decrease when the thickness of the backfill is increased. This effect can be attributed to the additional delay during their transport from the vault to the geosphere.

- The ADEs resulting from ^{14}C and ^{129}I are increased by increases in the values of man's total daily energy intake requirement and the dose conversion factors. Increased daily energy intake corresponds to the ingestion of more potentially contaminated food, water and air, and the ingestion pathway is the most important biosphere pathway that affects the critical group. Dose conversion factors are used to convert exposure to dose, and thus have a direct effect on the magnitude of the estimated doses.

Some of the above parameters, such as the half-life of ^{14}C, are accurately known physical constants. However other parameters could be influenced to some extent by modifications to the disposal facility, such as a vault design that would allow for a thicker backfill. Several of these changes were discussed in Section 6.2 for use as potential design constraints.

6.3.3.6 Summary of the Median-Value Sensitivity Analyses

This sensitivity analysis has identified parameters important to the maximum ADEs in a region of the parameter space centred near the median values. It shows that the tortuosity of the lower rock zone is the most important parameter for both small and large changes to parameter values. This parameter is one of several used to describe the movement of contaminants in the rock immediately surrounding the vault; others include the groundwater velocity scaling factor and the waste exclusion distance.

The results also show that the switch parameter that selects the source of domestic water is important: simulations involving the use of well water have larger ADEs than simulations involving lake water.

Sections D.6 to D.8 in Appendix D examine in detail the effects of all the important parameters listed in Tables 6-2, 6-3 and 6-4. This appendix also discusses several other parameters that are important when considering objective functions that isolate the performance of the vault, geosphere and biosphere.

As noted in Section 6.3.1, a main purpose of the analysis of the median simulation is to identify important features and processes in the system model and to understand why they are important. We use this information to guide the probabilistic analysis, because the the results of many randomly selected simulations are more difficult to unravel. In particular, we use results from the sensitivity analysis of the median-value simulation to help interpret the sensitivity analyses that take into consideration the simultaneous variation of all parameters over their entire ranges of possible values.

In developing a disposal facility, including site characterization and design studies, sensitivity analyses are expected to be an important tool in determining features of the site and design that are important to the performance of the system. These analyses can be used to determine whether and what additional studies should be carried out; for example, to better delineate features of the geosphere and engineered barriers. Sensitivity analyses, similar to those described in Section 6.2, can be used to develop design constraints to improve the margin of safety of the disposal system. Finally, other sensitivity analyses could contribute toward optimization of costs and safety of the disposal system.

6.4 ANALYSIS OF BARRIER EFFECTIVENESS

This section describes a special sensitivity analysis of the median-value simulation. It examines the relative effectiveness of several engineered and natural barriers that contribute to the safety of the reference disposal system evaluated in this postclosure assessment. The analysis is focussed on the main pathway that contributes to the ADEs for times up to 10^5 a: this pathway originates in vault sector 11, involves transport along fracture zone LD1, and enters the biosphere at the well.

The sequence of barriers affecting contaminant transport are illustrated in Figure 6-11. We examine eight barriers:

- the titanium container;
- the waste matrices (used fuel and Zircaloy);
- the buffer;

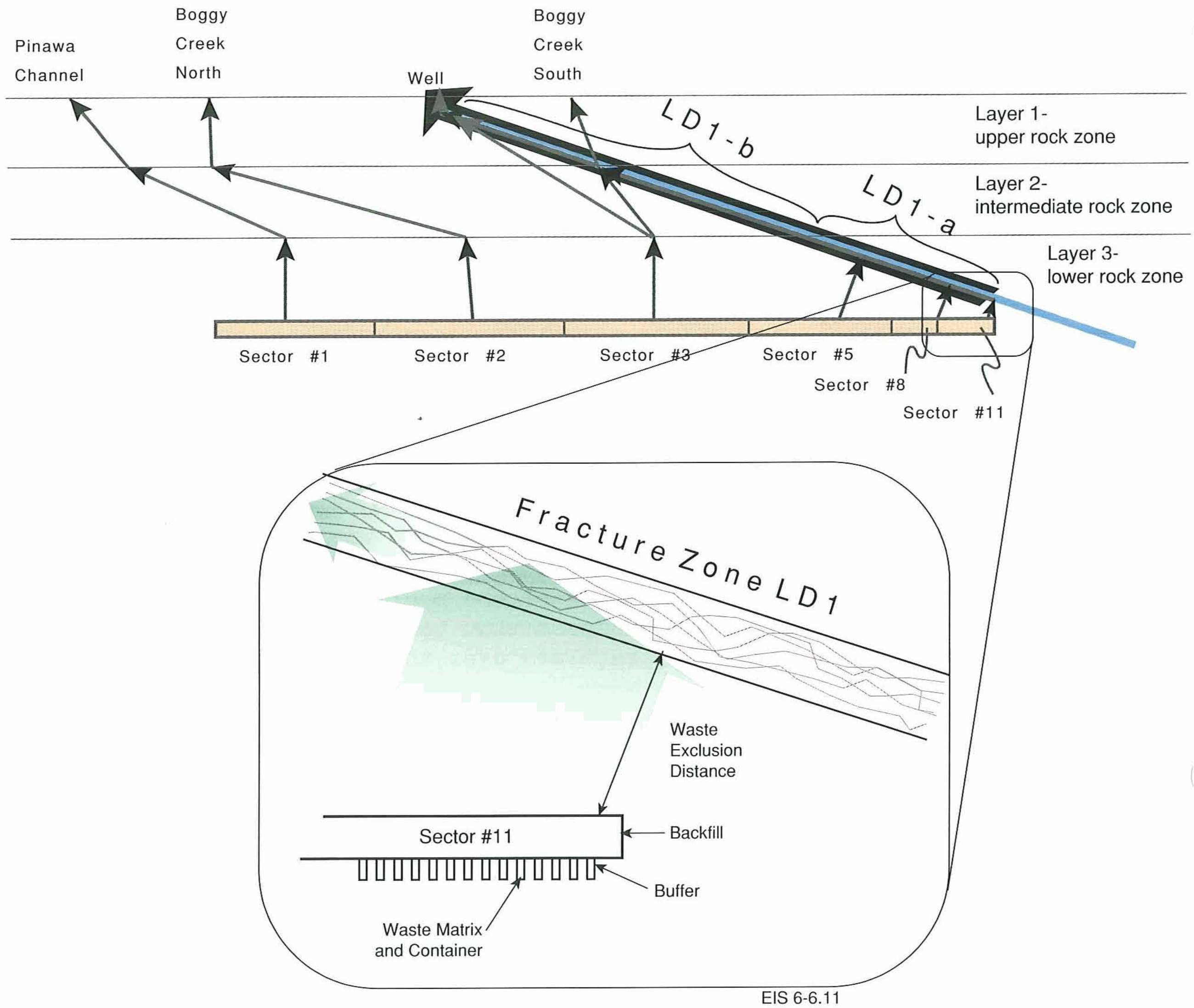

FIGURE 6-11: Barriers to Contaminant Transport in the Median-Value Simulation

This figure shows the principal pathways for contaminant transport from the vault to the biosphere; several important barriers occur along these pathways. An effective barrier is one that delays and attenuates the release of contaminants.

In the median-value simulation, the major pathway for contaminant transport originates at vault sector 11, involves transport along fracture zone LD1, and enters the biosphere at the well. The barriers considered along this pathway are the titanium container, waste matrices, buffer, precipitation (of technetium) in the buffer, backfill, the sparsely fractured rock within the waste exclusion distance and fracture zone LD1 leading from near the vault to the well. Two parts of the fracture zone are examined: LD1-a and LD1-b. Fracture zone LD1-a is approximately 540 m long and is located in the lower rock zone; LD1-b is approximately 780 m long and is located in the intermediate and upper rock zones.

- the backfill;
- precipitation of sparingly soluble elements in the buffer (our calculations show that only technetium would precipitate in the chemical environment represented by the median-value simulation);
- the rock within the waste exclusion distance (about 50 m of sparsely fractured rock) that isolates the waste emplacement part of any vault room in sector 11 from fracture zone LD1;
- the lower part of LD1, labelled LD1-a in Figure 6-11, which is in the lower rock zone and is about 540 m long; and
- the upper part of LD1, labelled LD1-b in Figure 6-11, which is in the intermediate rock and upper rock zones and is about 780 m long.

(Chemical precipitation takes into consideration the effect of electrochemical potential on element solubilities. It could be classified as an engineered barrier because we simulate the process within the buffer (Section 5.2), and it would be feasible to enhance precipitation in the buffer using suitable additives.)

An effective barrier is one that delays and attenuates contaminant release. Delayed releases may lead to smaller radiation doses because radioactive decay during the delay time may reduce the contaminant inventory and its subsequent discharge to the biosphere. (On the other hand, doses may be greater if ingrowth leads to larger inventories, and thus to larger discharges of a contaminant.) Attenuated releases lead to a decrease in the concentration of a released contaminant because the releases are dispersed in time or space.

The effects of delay and attenuation are generally inseparable. For example, there are more than 100 000 containers in the vault, and their net effect is both to delay and to attenuate the release of a radionuclide:

- A radionuclide cannot be released until the container has failed. This delay time may decrease significantly the inventory of a radionuclide and is especially effective for short-lived nuclides that do not have precursors. For example, if a container remains intact for 1000 a, then the surviving inventory of tritium (with a half-life of 12.4 a), would be about $2^{(1000/12.4)}$ or 10^{24} times smaller than its initial inventory.
- The entire surviving inventory of a radionuclide will not be released at the instant of failure of one container. Instead, the radionuclide will be released at different times from different containers because there is a distribution in time of the container failures (Section D.2 in Appendix D). This process has the effect of dispersing releases in time, with subsequent attenuation of releases at any particular time. Moreover, because the containers are dispersed throughout the disposal vault, the release of a radionuclide will also be dispersed in space. That is, its entire surviving inventory is not released at some point

source but instead at different locations throughout the vault. For the model of the reference disposal system, we use 12 sectors to represent the entire disposal vault (Sections 5.2 and 5.4). In the following analysis, we consider only containers in vault sector 11, and thus do not explicitly evaluate the effects of dispersion in space (although other analyses in Sections D.3 and D.4 in Appendix D show that 9 of the 12 vault sectors do not contribute to impacts even at 10^5 a).

We quantify the effectiveness of each barrier by calculating a barrier performance measure for each contaminant. The barrier performance measure is defined as follows:

$$\text{barrier performance measure} = \frac{\text{amount of contaminant exiting the barrier}}{\text{amount of contaminant entering the barrier}},$$

or the fraction of the contaminant released from the barrier. We calculate this measure as a function of time. Although relatively simple, this definition requires more detailed specification to avoid ambiguities and to permit comparison of different barriers. The required details are discussed in Section D.9.1 in Appendix D.

Figure 6-12 shows some performance measures as a function of time for ^{129}I:

- The rock within the 50-m waste exclusion distance is the most effective barrier in delaying and attenuating releases; for instance, the total fraction released from this barrier is less than 10^{-4} for times up to 2×10^4 a.

- The backfill and waste matrix (used fuel) are somewhat less effective, whereas the buffer, container and fracture zone are relatively unimportant. (More precisely, the used-fuel waste matrix is a very effective barrier for the congruently released ^{129}I but ineffective for the instantly released ^{129}I.)

- For times beyond about 6×10^4 a, the results show the waste matrix becomes more effective than the buffer. The results also indicate that, at times beyond 10^5 a, the waste matrix becomes the most effective barrier. The maximum in the total fraction released from the waste matrix (used fuel) is less than 0.1 and is virtually entirely due to the initial inventory of ^{129}I available for instant release. The instant-release inventory of ^{129}I is 8.1% in the median-value simulation (Section D.2 in Appendix D).

Section D.9.1 in Appendix D describes the results obtained for ^{14}C, ^{99}Tc and ^{238}U. Results for ^{14}C are similar to those for ^{129}I except that the effects of radioactive decay are important (Figure D-64 in Appendix D). Precipitation is an effective barrier for ^{99}Tc because it significantly reduces ^{99}Tc release from the buffer. However, the backfill is the most effective barrier for ^{99}Tc by many orders of magnitude (Figure D-65 in Appendix D). The rock within the waste exclusion distance is an extremely effective barrier for ^{238}U (Figure D-66 in Appendix D). The used-fuel matrix is also an effective barrier for ^{238}U because its release involves only the congruent-release mechanism.

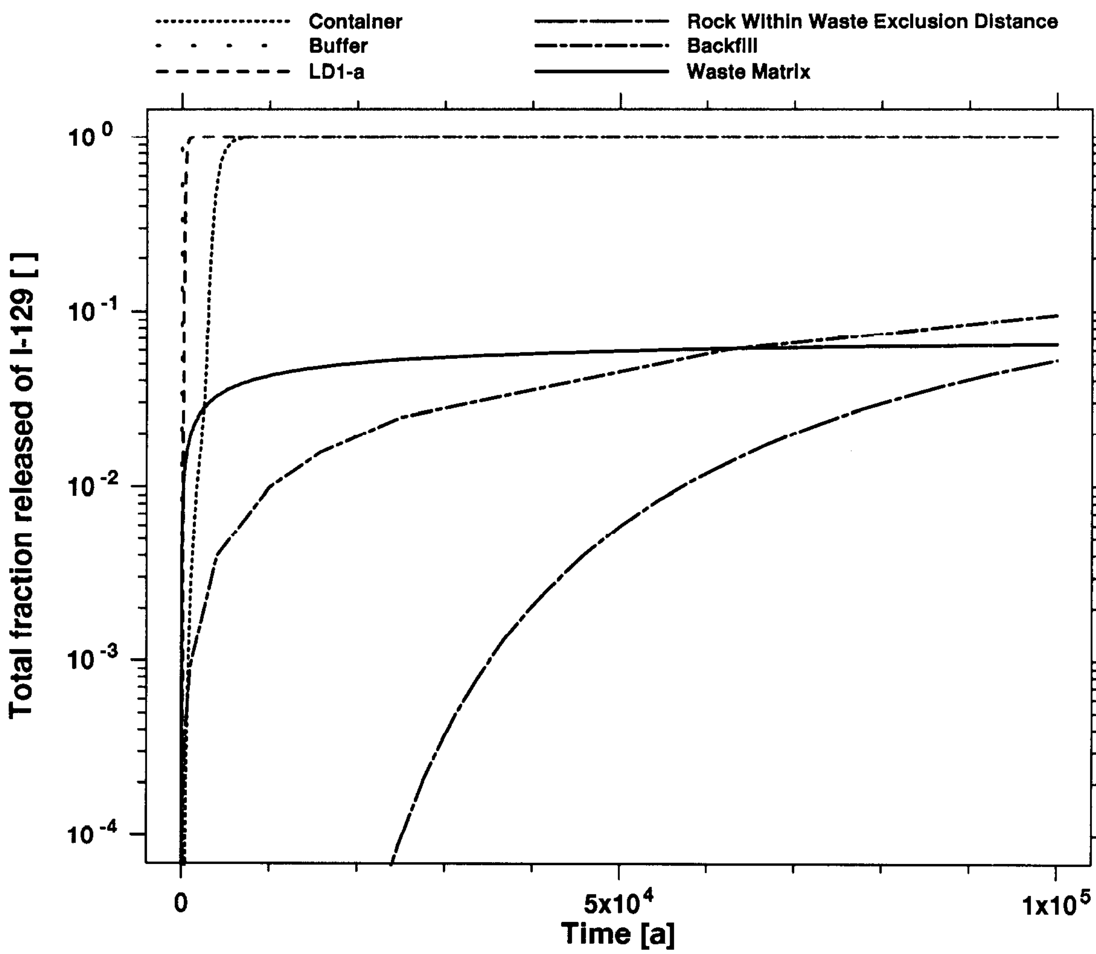

FIGURE 6-12: Barrier Performance Measures for ^{129}I from Used Fuel

The curves are calculated from the models for six barriers: the used-fuel waste matrix, container, buffer, backfill, rock within the waste exclusion distance and the lower (LD1-a) part of fracture zone LD1. The calculations assume that a unit amount of ^{129}I is instantaneously input to the barrier at time equal to zero; the curves show the total fraction (integrated over time) released as a function of time. The vertical axis uses a logarithmic scale and plots the total fraction released from the barrier or the performance measure of the barrier for ^{129}I.
The most effective barriers for ^{129}I are the rock within the waste exclusion distance, followed by the backfill and waste matrix.

The barriers are independent of one another and act in sequence to control contaminant release. We can obtain a simple estimate of their sequential effect from the product of the fractions released from each of the eight barriers. We use this product to define a net fraction released. In fact, this definition is very pessimistic because of the way in which we calculate the fractions released from each barrier. For each barrier, we calculate the fraction released assuming a unit amount of contaminant is instantaneously input at time equal to zero. In reality, the output from the first barrier would be the input to the second barrier (and so forth). In general, the output from the first barrier would not be a unit amount at an instant in time; rather the output would be both delayed and attenuated. Accordingly, the input to the second barrier would be a smaller amount of contaminant, spread over some longer time frame. Thus the net fraction released, as defined above, greatly overestimates the actual release from a sequential combination of barriers. (The results from SYVAC3-CC3 described in all other sections of this report do take into account the sequential effects of the barriers.)

The net fraction released is thus a pessimistic overestimate of the fraction that could be released. For ^{129}I the maximum possible fraction released is 6×10^{-5} for times up to 6×10^{4} a. The sequential arrangement of barriers gives rise to a much larger reduction in release than for any barrier acting individually.

Table 6-5 summarizes the net fractions released up to 10^5 a for 14 radionuclides and chemically toxic elements that have the largest net fraction released. The smallest value listed is 2×10^{-34} for ^{93}Mo from used fuel. For all other contaminants shown in Tables 5-3 and 5-4 and not listed in Table 6-5, the calculated net fractional release is less than 9×10^{-38}. Table 6-5 also shows the net fractions released for each contaminant from a sequential combination of the eight barriers. The table illustrates, for example, that at 10^5 a bromine has a maximum possible fraction released of 3×10^{-4}, and its three most effective barriers are the rock within the waste exclusion distance, the waste matrix (used fuel) and the backfill.

Figures 6-13 and 6-14 summarize the performance of the barriers for most of the radionuclides and nine chemically toxic elements considered in the postclosure assessment. The two figures show results at 10^4 a and at 10^5 a respectively. Both figures are constructed using a logarithmic transformation affecting the lengths of the boxes (details are given in Section D.9.2 in Appendix D). The length of a box is indicative of the effectiveness of the barrier for a contaminant:

- A box length of zero indicates a relatively ineffective barrier. It corresponds to a barrier that releases all the contaminant over 10^4 or 10^5 a (its barrier performance measure is unity). All entries, except for ^{99}Tc, have a box length of zero in the column labelled "Precipitate in Buffer".

- Longer boxes indicate that a barrier is more effective in attenuating and delaying a contaminant release. For an extremely effective barrier, the calculated fraction of a contaminant released (or the performance measure) is 0. The box lengths for ^{241}Pu releases from the backfill in both figures represent this small fraction.

TABLE 6-[illegible]

FRACTIONAL RELEASES FROM BARRIERS*

Nuclide		Net Fraction Released	Total Fraction Released from Barrier 1	Barrier 2	Barrier 3	Barrier 4	Barrier 5	Barrier 6	Barrier 7	Barrier 8
Br	F	3 x 10^{-4}	5 x 10^{-2} ex	6 x 10^{-2} wa	1 x 10^{-1} ba	1 x 10^{0} pr	1 x 10^{0} Lb	1 x 10^{0} bu	1 x 10^{0} La	1 x 10^{0} co
^{129}I	F	3 x 10^{-4}	5 x 10^{-2} ex	6 x 10^{-2} wa	1 x 10^{-1} ba	1 x 10^{0} pr	1 x 10^{0} Lb	1 x 10^{0} co	1 x 10^{0} bu	1 x 10^{0} La
^{81}Kr	F	1 x 10^{-4}	4 x 10^{-2} ex	8 x 10^{-2} ba	8 x 10^{-2} wa	4 x 10^{-1} bu	1 x 10^{0} co	1 x 10^{0} Lb	1 x 10^{0} La	1 x 10^{0} pr
^{14}C	F	7 x 10^{-9}	7 x 10^{-5} ex	8 x 10^{-3} ba	6 x 10^{-2} wa	6 x 10^{-1} La	6 x 10^{-1} Lb	6 x 10^{-1} co	1 x 10^{0} bu	1 x 10^{0} pr
^{210m}Bi	Z	3 x 10^{-13}	2 x 10^{-7} wa	4 x 10^{-3} ba	7 x 10^{-3} bu	5 x 10^{-2} ex	1 x 10^{0} co	1 x 10^{0} pr	1 x 10^{0} Lb	1 x 10^{0} La
^{208}Bi	Z	2 x 10^{-13}	2 x 10^{-7} wa	4 x 10^{-3} ba	6 x 10^{-3} bu	5 x 10^{-2} ex	1 x 10^{0} co	1 x 10^{0} Lb	1 x 10^{0} La	1 x 10^{0} pr
Sb	F	9 x 10^{-15}	6 x 10^{-9} wa	4 x 10^{-3} ba	7 x 10^{-3} bu	5 x 10^{-2} ex	1 x 10^{0} pr	1 x 10^{0} Lb	1 x 10^{0} La	1 x 10^{0} co
^{14}C	Z	7 x 10^{-15}	6 x 10^{-8} wa	7 x 10^{-5} ex	8 x 10^{-3} ba	6 x 10^{-1} La	6 x 10^{-1} Lb	6 x 10^{-1} co	1 x 10^{0} bu	1 x 10^{0} pr
^{99}Tc	F	2 x 10^{-17}	6 x 10^{-8} ba	4 x 10^{-3} pr	1 x 10^{-3} bu	1 x 10^{-3} ex	6 x 10^{-2} wa	9 x 10^{-1} La	9 x 10^{-1} Lb	1 x 10^{0} co
^{187}Re	Z	4 x 10^{-20}	8 x 10^{-8} ba	2 x 10^{-7} wa	1 x 10^{-3} bu	2 x 10^{-3} ex	1 x 10^{0} pr	1 x 10^{0} Lb	1 x 10^{0} La	1 x 10^{0} co
Mo	F	3 x 10^{-20}	6 x 10^{-9} wa	8 x 10^{-8} ba	1 x 10^{-3} bu	5 x 10^{-2} ex	1 x 10^{0} pr	1 x 10^{0} Lb	1 x 10^{0} La	1 x 10^{0} co
^{99}Tc	Z	1 x 10^{-20}	6 x 10^{-8} ba	2 x 10^{-7} wa	1 x 10^{-3} bu	1 x 10^{-3} ex	9 x 10^{-1} La	9 x 10^{-1} Lb	1 x 10^{0} co	1 x 10^{0} pr
^{39}Ar	F	4 x 10^{-31}	5 x 10^{-20} ex	4 x 10^{-4} ba	8 x 10^{-4} co	2 x 10^{-3} bu	8 x 10^{-2} wa	4 x 10^{-1} La	4 x 10^{-1} Lb	1 x 10^{0} pr
^{93}Mo	Z	8 x 10^{-33}	1 x 10^{-13} ba	5 x 10^{-8} wa	9 x 10^{-7} bu	5 x 10^{-6} ex	5 x 10^{-1} co	9 x 10^{-1} La	9 x 10^{-1} Lb	1 x 10^{0} pr
^{107}Pd	F	3 x 10^{-33}	1 x 10^{-22} ex	6 x 10^{-9} wa	3 x 10^{-2} ba	1 x 10^{-1} bu	1 x 10^{0} La	1 x 10^{0} Lb	1 x 10^{0} pr	1 x 10^{0} co
^{237}Np	F	4 x 10^{-34}	7 x 10^{-16} ex	6 x 10^{-9} wa	8 x 10^{-8} ba	1 x 10^{-3} bu	1 x 10^{0} La	1 x 10^{0} Lb	1 x 10^{0} co	1 x 10^{0} pr
^{93}Mo	F	2 x 10^{-34}	1 x 10^{-13} ba	1 x 10^{-9} wa	9 x 10^{-7} bu	5 x 10^{-6} ex	5 x 10^{-1} co	9 x 10^{-1} La	9 x 10^{-1} Lb	1 x 10^{0} pr

* This table compares the effectiveness of eight barriers for different contaminants at 10^5 a. Smaller fractions indicate that a barrier is more effective.

Contaminants are identified in the first column, with "F" and "Z" indicating the used-fuel and Zircaloy waste matrices. There are 17 entries, but ^{14}C, ^{93}Mo and ^{99}Tc appear twice, once for each matrix. Contaminants in Tables 5-3 and 5-4 not listed here have net fractional releases less than 9 x 10^{-38}, the smallest positive number that was possible in the calculations. (We report all calculated values for completeness, recognizing that some small numbers could represent a minute fraction of an atom).

Contaminants are ranked downwards in decreasing order of the net fraction released (second column), a pessimistic estimate of the releases to 10^5 a that could occur from a sequential combination of independent barriers. It is calculated as the product of the fractions released from the eight barriers. Columns 3 through 10 show total fractions released from different barriers, ranked across a row in increasing order. The following abbreviations identify the individual barriers:

- ba = backfill;
- bu = buffer;
- co = container;
- ex = rock within the waste exclusion distance;
- La = lower part (LD1-a) of fracture zone LD1;
- Lb = upper part (LD1-b) of fracture zone LD1;
- pr = precipitation (for ^{99}Tc) and
- wa = waste matrix.

The most consistently effective barriers are the rock within the waste exclusion distance, the waste matrices (used fuel and Zircaloy) and the backfill: their fractional releases are less than 0.1 for all contaminants.

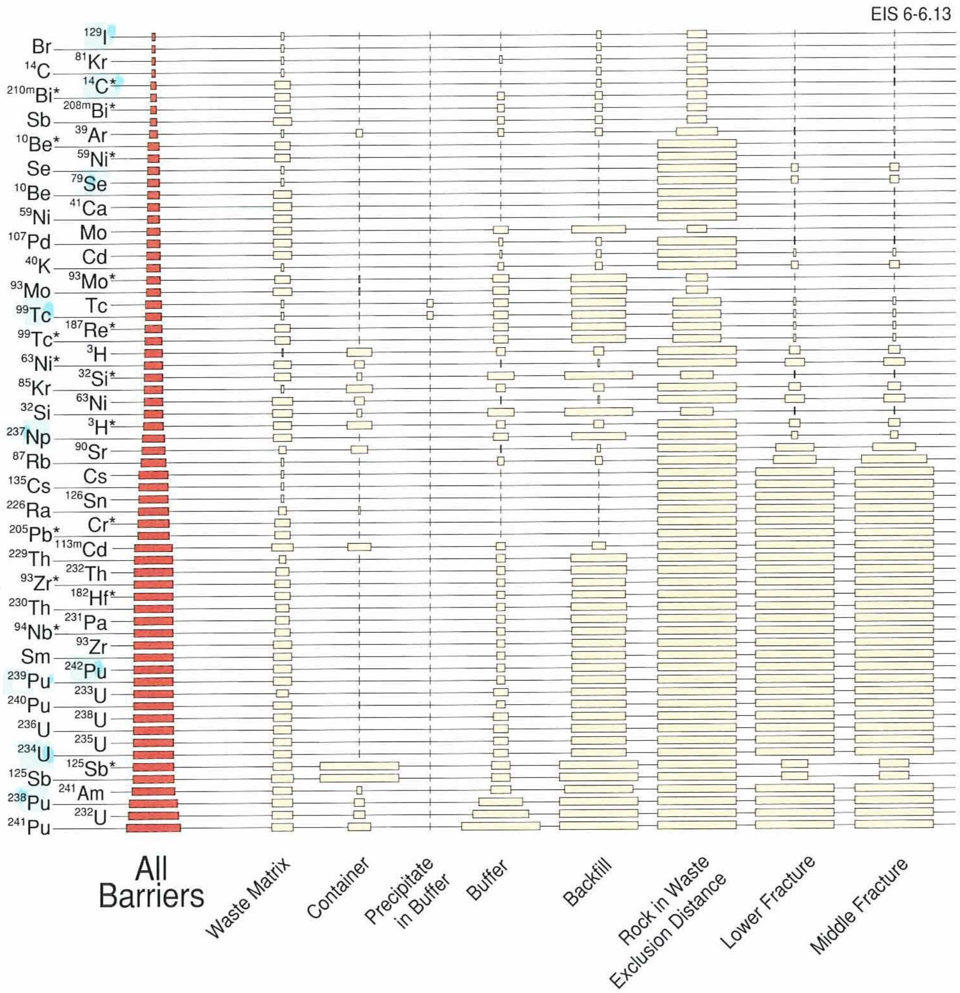

FIGURE 6-13: Summary of the Analysis of Barrier Performance at 10^4 a

This figure illustrates the relative effectiveness of eight barriers at 10^4 a after closure of the disposal vault. The labels on the left-hand side of the figure identify different contaminants, with "*" indicating contaminants associated with the Zircaloy matrix (all others are from the used-fuel matrix).
The eight columns on the right of the figure illustrate the effectiveness of the eight barriers, each considered separately, and the first column of boxes represents a pessimistic estimate of the net effectiveness of a sequential combination of the eight barriers. The length of each box represents the effectiveness of a barrier: a longer box corresponds to greater attenuation and delay or to a smaller fractional release of a contaminant. The smallest possible length is zero (such as "Precipitate in the Buffer" for ^{129}I), corresponding to an ineffective barrier with a fractional release of unity at 10^4 a. The longest possible box (such as the five on the right for ^{241}Pu) represents an extremely effective barrier, with a fractional release of 0 at 10^4 a. Calculation of these lengths involves a logarithmic transformation (Section D.9.2 in Appendix D).

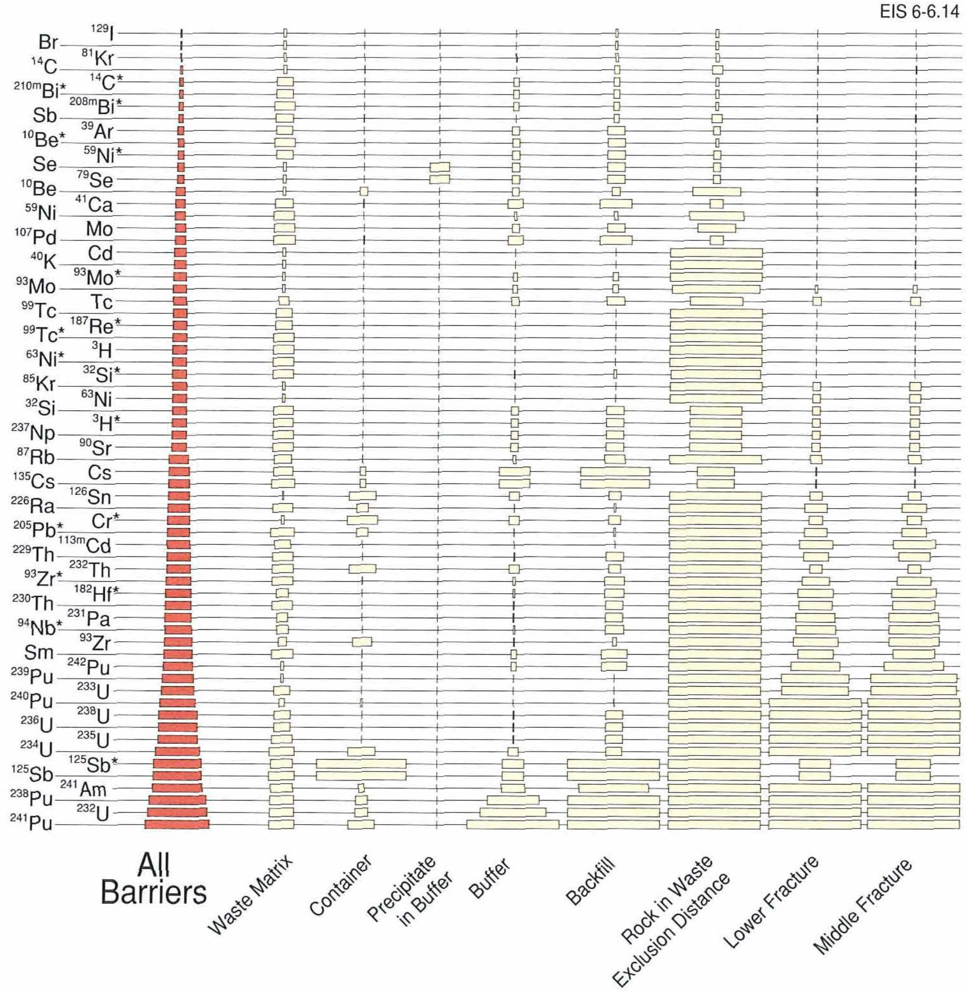

FIGURE 6-14: Summary of the Analysis of Barrier Performance at 10^5 a. Comments are as for Figure 6-13, except the time considered is 10^5 a.

The first column of boxes in Figures 6-13 and 6-14 shows the minimum possible effectiveness of a sequential combination of the eight barriers. The lengths of these boxes also use a logarithmic transformation (Section D.9.2 in Appendix D) applied to the net fraction released. Contaminants are ranked in the figures according to these lengths: contaminants near the bottom of the list, with longer boxes, are more attenuated and delayed than contaminants near the top of the list.

The results in Figures 6-13 and 6-14 can be used to compare the effectiveness of different barriers for different contaminants. The figures show that

- The effectiveness of a barrier is both nuclide-dependent and time-dependent.

- The radionuclides near the top of the figures are least affected by the sequence of barriers. Two of them, ^{14}C and ^{129}I, are the major contributors to ADEs (discussed in Section 6.3.2). Note that the rankings in Figures 6-13 and 6-14 are not the same as a ranking based on contributions to the total ADE because the calculations of the ADE include additional factors, such as radionuclide inventory, radiotoxicity and transport in the biosphere. For instance, ^{81}Kr is not an important contributor to the ADE because it has a relatively small inventory and is not significantly radiotoxic for most exposure pathways.

- The chemically toxic elements near the top of the figures also have the largest estimated concentrations in the biosphere (Section 6.3.2). Bromine occurs first in both instances, followed by antimony. Note, however, that the rankings in Figures 6-13 and 6-14 do not include factors such as contaminant inventory and transport in the biosphere.

- Small amounts of only a few radionuclides are likely to pass through all barriers and reach the biosphere in 10^4 or 10^5 a. The most likely candidates are ^{129}I, ^{81}Kr, ^{14}C, ^{210m}Bi and ^{208}Bi. Of these, ^{210m}Bi and ^{208}Bi have at least one very effective barrier. Technetium-99 and ^{187}Re and all the contaminants below them have two or more barriers that are extremely effective.

- For the bismuth isotopes, ^{14}C from Zircaloy and ^{99}Tc from Zircaloy, the Zircaloy waste matrix is an effective barrier. This occurs because releases from Zircaloy are limited to congruent release controlled by the low solubility of the Zircaloy matrix (1.79×10^{-6} mol/m^3 in the median-value simulation).

- The used-fuel and Zircaloy waste matrices are effective barriers for contaminants that are released congruently. For the used-fuel waste matrix, these contaminants include the isotopes of plutonium and all other actinides, and most of the initial inventory of ^{129}I and ^{14}C.

- The container is very effective for radionuclides with short half-lives, for example, tritium (^3H) and ^{125}Sb.

- Chemical precipitation in the buffer is important only for ^{99}Tc from the used-fuel waste matrix; Technetium-99 from Zircaloy does not reach the solubility limit for technetium. (Ideally, ^{99}Tc from used fuel and Zircaloy should be modelled together because they are chemically identical. However, modelling them separately is much simpler and is conservative in the sense that it overestimates releases of ^{99}Tc from the buffer.)

- The buffer, backfill and fracture zone LD1 are effective barriers for contaminants that tend to sorb strongly.

- The rock within the waste exclusion distance is an extremely effective barrier. It limits the releases of more than half the contaminants to a negligible fraction.

In summary, the results in Figures 6-13 and 6-14 suggest that, for the median-value simulation, only small amounts of a few contaminants are likely to reach the biosphere in 10^4 and 10^5 a: bromine, ^{129}I, ^{81}Kr and ^{14}C. Of these, the analysis in Section 6.3.2 shows that two largest releases to the biosphere are from bromine and ^{129}I, followed by ^{14}C with much smaller releases. All other contaminants have one or more very effective barriers, with the rock within the waste exclusion distance being most often the most effective.

This analysis has also been carried out for vault sector 1 of the median-value simulation. The net fractional releases are more than 10 orders of magnitude smaller for ^{129}I and ^{81}Kr from sector 1, supporting the previous observation that the main pathway contributing to estimated dose originates in vault sector 11.

6.5 RESULTS FROM THE PROBABILISTIC ANALYSIS

6.5.1 Introduction to the Probabilistic Analysis

In the probabilistic assessment, several thousands of simulations are analyzed, with each simulation using a set of randomly selected values for the parameters of the system model:

- We analyzed results from 40 000 simulations for seven of the radionuclides in Table 5-4 that are expected to cause the largest radiation doses over times up to 10^5 a following closure of the vault. They are ^{14}C, ^{135}Cs, ^{129}I, ^{59}Ni, ^{107}Pd, ^{79}Se and ^{99}Tc from used fuel. Subsequent analyses confirmed that no other radionuclide makes a significant contribution to the total radiation dose over 10^5 a (in fact our results show that we could further reduce the seven radionuclides to include only ^{14}C and ^{129}I). Moreover, convergence of the results from 40 000 simulations is satisfactory because we can calculate robust and relatively precise statistical arithmetic averages and show that these averages are clearly below regulatory criteria.

- We also analyzed results from at least 2000 simulations for all the other radionuclides and each of the nine chemically toxic elements listed in Tables 5-3 and 5-4 (Section 5.9).

Each simulation uses random sampling (also known as Monte Carlo sampling) to select a parameter value from its range of possible values. In making these random samples, we use a random number generator (with no re-use of random seeds) to select a uniform random variate between 0 and 1. We then use a transformation, known as the inverse cumulative distribution method (Knuth 1969; Rubinstein 1981), to determine the corresponding parameter value from its PDF. The SYVAC3-CC3 parameters are described using the following PDF types: normal, lognormal, uniform, piecewise uniform, loguniform, triangular, beta, and constant (Figure A-6 in Appendix A gives sample plots).

The probabilistic approach includes the effects of parameter uncertainty, and the importance of these effects is illustrated in Figure 6-15. This figure shows curves of ADEs from ^{129}I versus time from five simulations

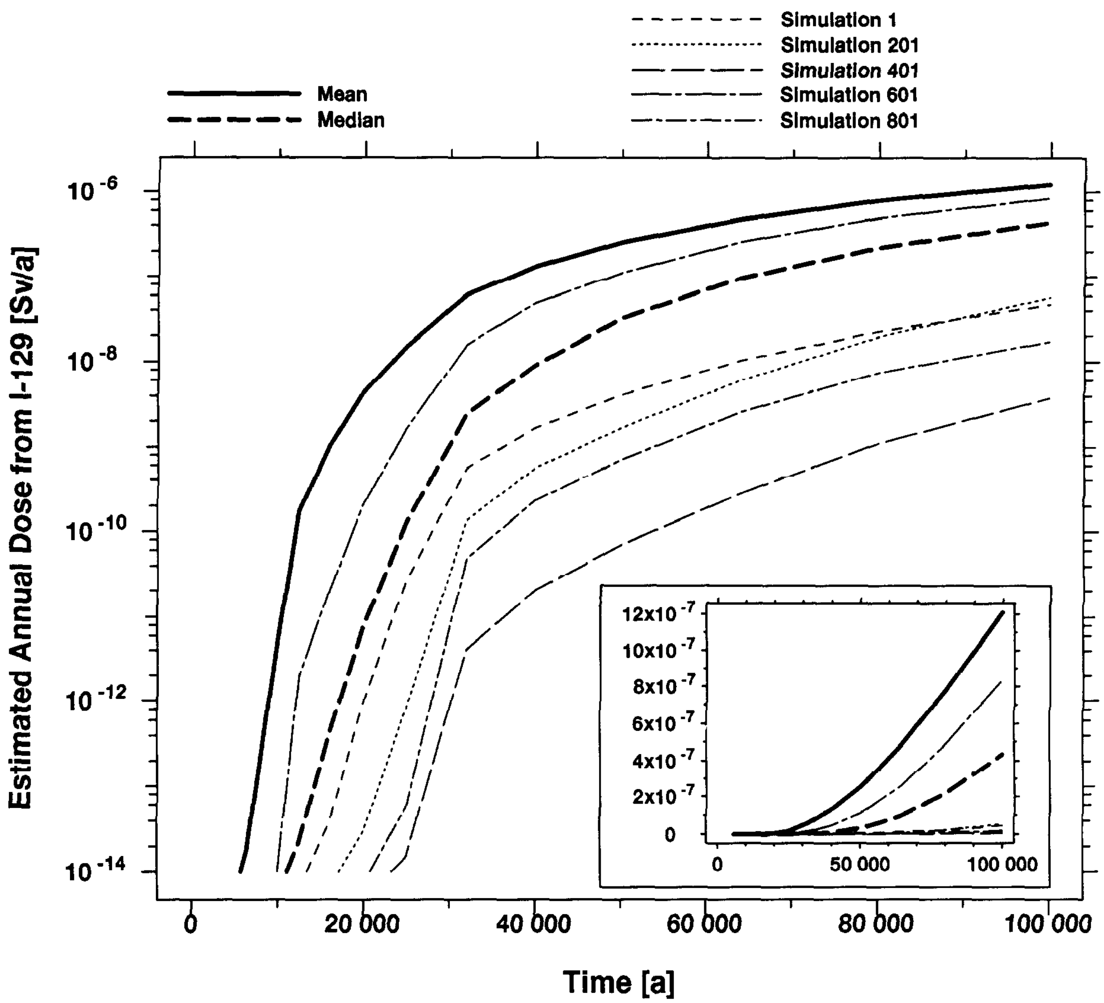

FIGURE 6-15: Curves of Estimated Annual Dose from ^{129}I Versus Time

The inset shows the same curves with linear vertical scales; the larger figure uses a logarithmic vertical scale to better distinguish the curves over a large range of annual dose estimates (ADEs). Five curves are plotted for simulations with randomly selected parameter values: simulation numbers 1, 201, 401, 601 and 801 from the first 1000 randomly sampled simulations. The wide range of ADEs is caused by the uncertainty in the parameters of the system model. The curve labeled "mean" is the arithmetic average of the 1000 simulations. It lies above the curves for simulations 1, 201, 401, 601 and 801 (but cannot lie above all curves from all the 1000 randomly selected simulations) because the arithmetic average is dominated by a few simulations that have large ADEs. The curve labelled "median" is the annual dose curve obtained for a special simulation: it is the median-value simulation, discussed in Section 6.3, for which all parameters are fixed at their median values.

with randomly selected parameter values and from the median-value simulation. It also shows the curve for the mean ADE versus time, where the mean is the arithmetic average from 1000 randomly selected simulations. The figure demonstrates that

- There is a wide variation in the ADE caused by the uncertainty in the parameter values used to describe the performance of the disposal system.

- The mean ADE curve lies above the other curves in the figure. At each point in time, the mean ADE is the arithmetic average of 1000 estimates of annual dose. Note that the mean ADE curve cannot lie above all of the ADE curves for the 1000 randomly sampled simulations. If curves were plotted for all of these simulations, most would lie below the mean, but a few would be above.

Because these estimates range over many orders of magnitude, the arithmetic average is dominated by the largest values. Figure 6-15 shows a case where the ADEs at 10^5 a are approximately 10^{-9} Sv/a from simulation 401, 10^{-8} Sv/a/a from simulations 1, 201 and 801, and 10^{-6} Sv/a from simulation 601. The average of these five estimates is about 0.2×10^{-6} Sv/a; that is, the contributions to the average from simulations 1, 201, 401 and 801 are dominated by the contribution from simulation 601.

The figure also shows the ADE curve from the median-value simulation. Clearly this single simulation does not represent the entire range of ADEs, nor does it give an accurate approximation to the mean ADE curve. As noted earlier, we examine the median-value simulation principally because we can trace in detail the functioning of the system model and gain insight into its operations and interactions. We can also perturb values of parameters and identify the most influential parameters based on a fixed reference simulation. In contrast, the mean ADE curve does not correspond to any single simulation in particular. We cannot use the mean ADE curve to investigate questions, such as "What was the release of ^{129}I from vault sector 12?" because the answer varies from simulation to simulation.

We use the arithmetic average of the ADE from a large number of randomly selected simulations for comparison with regulatory criteria. In fact, the AECB (1987a) specifies the arithmetic average for use in the radiological risk equation when using a probabilistic analysis (Section 1.4.1 and Appendix C). The arithmetic average has four important properties.

- It is computed using all values, and thus represents the entire group of values.

- It approaches a limiting value as the number of values increases, and the limit is the mean of the underlying distribution. This result follows from the central-limit theorem: "As sample size increases, the means of samples drawn from a population of any distribution will approach the normal distribution" (Sokal and Rohlf 1981), and the mean of this normal distribution is equal to the mean of the underlying distribution.

- It is additive: the arithmetic mean doses for two different radionuclides can be added to get a mean dose for both radionuclides, and arithmetic means from two sets of simulations can be averaged to get a mean for both sets.

- It is an estimate of statistical expectation, accounting for the uncertainties in all parameters.

Of course, the arithmetic average is just one way of describing the distribution of ADEs at any time. From the set of simulation results, we can estimate the distribution itself and any other statistics, such as the 99th percentile. The distribution, however, is rather difficult to represent mathematically because (as shown in Section 6.5.2) it is highly skewed, such that the vast majority of ADE values at any point in time are smaller than the average value at that time, and the average tends to be dominated by a few simulations with relatively large ADEs.

In addition, many other measures of the centre of the distribution of ADEs would be less conservative for the results from SYVAC3-CC3 because the distribution is so highly skewed. For example, for a set of n values that represent this distribution, the median of the set (approximately the n/2 largest value), its mode (the most frequent value), and its geometric mean (the n^{th} root of the product of the n values) are all much smaller than its arithmetic average (the sum of the n values divided by n).

The above discussion also applies to other calculated variables of interest. We, therefore, report arithmetic averages for variables such as estimated concentrations of contaminants in the biosphere and ADEs to nonhuman biota.

Table 6-6 contains examples of arithmetic averages. It summarizes the averaged fate of selected contaminants at 10^5 a, computed from 1000 simulations. At 10^5 a, most of the contaminants remain in the vault and are still located within the used fuel or Zircaloy. Only a few contaminants reach the geosphere, and fewer still discharge to the biosphere in any appreciable quantities. Discharges to the biosphere, over 10^5 a, are largest for

- the chemically toxic elements bromine and antimony (from used fuel); and

- the radionuclides ^{14}C (from both used fuel and Zircaloy), ^{129}I (used fuel) and ^{81}Kr (used fuel).

Similar overall results are discussed in Table 6-1 for the median-value simulation. However, a detailed comparison of the two tables suggests that contaminants have moved somewhat farther and in greater quantities when comparing the arithmetic averages with the median values.

Figure 6-16 helps to explain why this is so by showing estimated values of the total amount of ^{129}I discharged to the biosphere from 1000 randomly sampled simulations. These simulations yield a wide distribution of values. For many simulations, the estimated values are close to the estimated value of 0.28 mol from the median-value simulation. However, the

TABLE 6-6

AVERAGE AMOUNTS OF SELECTED CONTAMINANTS AT VARIOUS LOCATIONS AT 10^5 a

Radio-Nuclide/ Toxic Element	Average Initial Inventory (mol)	Average Amount in Containers at 10^5 a (mol)	Average Amount in Buffer at 10^5 a (mol)	Average Amount in Backfill at 10^5 a (mol)	Average Amount in Vault at 10^5 a (mol)	Average Vault Release to 10^5 a (mol)	Average Amount in Geosphere at 10^5 a (mol)	Average Amount Released to Biosphere at 10^5 a (mol)
^{208}Bi Z	3.2×10^{-5}	2.6×10^{-5}	3.9×10^{-7}	8.6×10^{-9}	2.7×10^{-5}	5.9×10^{-11}	5.6×10^{-11}	4.6×10^{-15}
^{210m}Bi Z	5.2×10^{-4}	5.0×10^{-4}	7.1×10^{-6}	1.6×10^{-7}	5.1×10^{-4}	8.5×10^{-10}	8.4×10^{-10}	5.6×10^{-14}
Br	2.3×10^{4}	2.1×10^{4}	2.1×10^{-1}	1.1×10^{3}	2.2×10^{4}	2.2×10^{2}	2.2×10^{2}	2.0×10^{-1}
^{14}C	6.1×10^{3}	2.7×10^{-2}	2.6×10^{-6}	6.1×10^{-3}	3.3×10^{-2}	4.4	9.5×10^{-4}	3.9×10^{-5}
^{14}C Z	1.1×10^{3}	6.1×10^{-3}	9.8×10^{-9}	7.1×10^{-5}	6.2×10^{-3}	3.0×10^{-2}	7.3×10^{-6}	6.3×10^{-8}
^{135}Cs	3.0×10^{4}	2.7×10^{4}	5.2×10^{-3}	6.7×10^{-1}	2.7×10^{4}	2.8×10^{3}	2.7×10^{3}	0.0
^{129}I	6.1×10^{4}	5.7×10^{4}	1.3	3.3×10^{3}	6.0×10^{4}	6.1×10^{2}	6.1×10^{2}	1.0
^{81}Kr	1.2×10^{-2}	7.7×10^{-3}	9.5×10^{-5}	5.7×10^{-4}	8.4×10^{-3}	1.2×10^{-4}	1.0×10^{-4}	1.1×10^{-7}
Mo	1.7×10^{6}	1.7×10^{6}	1.4×10^{2}	3.4×10^{-2}	1.7×10^{6}	5.9×10^{-9}	5.9×10^{-9}	2.4×10^{-14}
^{59}Ni	1.2×10^{3}	4.8×10^{2}	1.3×10^{-4}	1.2×10^{-3}	4.8×10^{-2}	3.8×10^{-2}	2.3×10^{-2}	$<10^{-20}$
^{107}Pd	1.8×10^{5}	1.8×10^{5}	7.0×10^{-1}	3.0	1.8×10^{5}	9.7	9.6	6.1×10^{-16}
^{187}Re Z	9.4×10^{2}	9.3×10^{2}	6.5	2.8×10^{-2}	9.4×10^{2}	1.9×10^{-9}	1.9×10^{-9}	4.2×10^{-19}
Sb	6.8×10^{3}	6.8×10^{3}	3.4×10^{-1}	1.1×10^{-2}	6.8×10^{3}	7.3×10^{-5}	7.3×10^{-5}	5.2×10^{-10}
^{79}Se	3.4×10^{3}	1.1×10^{3}	1.2×10^{-4}	0.0	1.1×10^{3}	2.0×10^{2}	7.9×10	$<10^{-20}$
^{99}Tc	3.6×10^{5}	2.4×10^{5}	1.7×10^{4}	2.0×10^{2}	2.6×10^{5}	5.1×10^{-5}	4.9×10^{-5}	7.8×10^{-12}
^{99}Tc Z	9.0	6.4	8.2×10^{-2}	2.1×10^{-4}	6.5	3.0×10^{-11}	2.9×10^{-11}	1.7×10^{-20}

This table shows the arithmetic averages of the amounts of contaminants at various locations, taken from 1000 randomly sampled simulations. (The contaminants listed include those from Table 6-1 with the largest discharges to the biosphere.) The first column identifies the contaminants, with a "Z" indicating that the contaminant is from the Zircaloy waste matrix (all others are from the used-fuel (UO_2) waste matrix). The second column gives their average initial inventories. Columns 3, 4 and 5 show the average amounts in the containers (including the used fuel and Zircaloy waste matrices), buffer and backfill at 10^5 a. These amounts are summed in column 6, giving the average amounts in the vault. Column 7 lists the averages of the total amounts released from the vault for times up to 10^5 a. The last two columns describe the average amounts in the geosphere and the average amounts discharged to the biosphere. Entries of 0.0 indicate that the calculated value is less than 10^{-37} (a number related to precision of the computer).

At 10^5 a, most of the contaminants remain within the vault. Total discharges over 10^5 a to the biosphere exceed 10^{-10} mol only for Br, ^{14}C, ^{129}I, ^{81}Kr and Sb. Table 6-1 shows similar results from the median-value simulation.

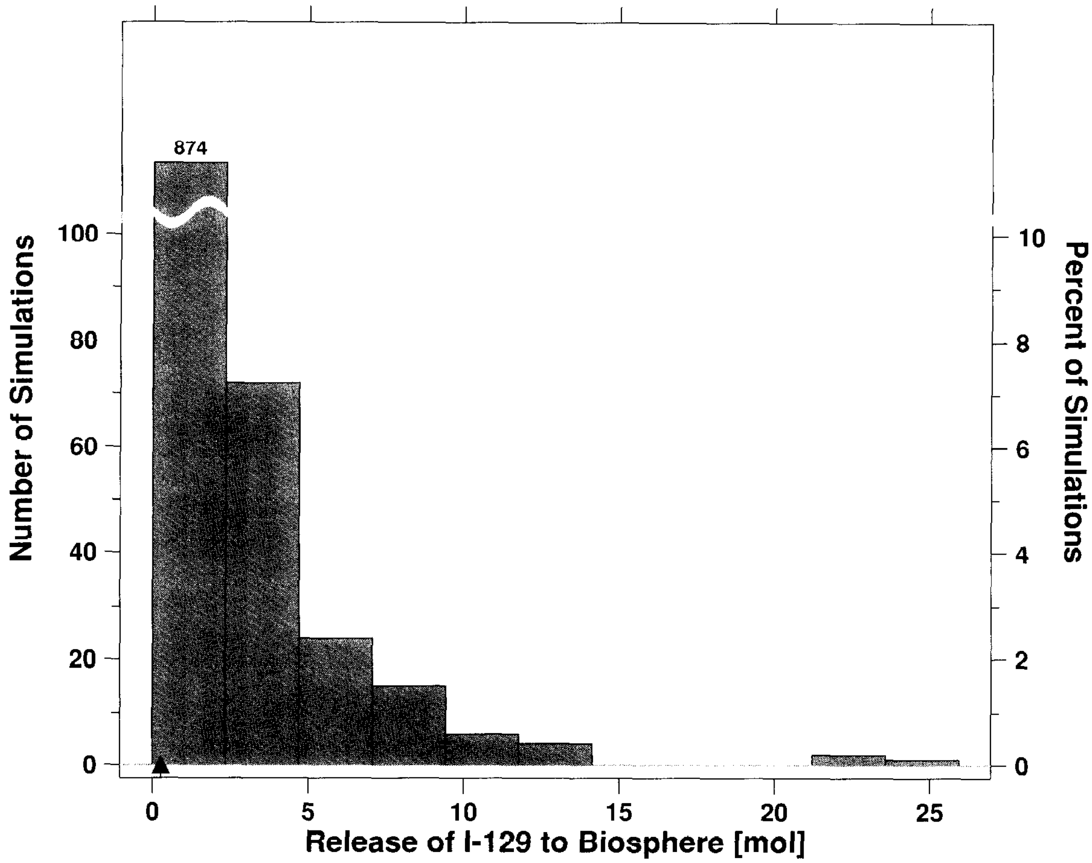

FIGURE 6-16: The Distribution of Amounts of ^{129}I Discharged to the Biosphere at 10^5 a

This plot shows results from 1000 simulations in which all parameters are sampled randomly from their associated probability density functions (PDFs). The uncertainties represented by these PDFs are reflected by the range of estimates for the total amount of ^{129}I released from the geosphere to the biosphere at 10^5 a. The arrow shows the corresponding estimate obtained from the median-value simulation (0.28 mol). Many estimates are close to that of the median-value simulation, but a few are much larger, so that the average released is 1.0 mol. Note the break in the vertical axis and in the first interval: there are 874 simulations in the first interval, and only about 70 in the second.

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distribution of results is skewed and a few simulations have very large values. The frequencies of occurrence of values is such that the arithmetic average is 1.0 mol, somewhat larger than the value from the median-value simulation.

In general, the distribution of results for any estimated variable is a function of the underlying uncertainty. Thus the largest relative differences between results in Tables 6-1 and 6-6 tend to occur with the amounts released to the biosphere because this variable reflects the underlying uncertainties in the vault and geosphere models. Similar effects are discussed in the following section for the distribution of ADEs.

In the remainder of Section 6.5, we discuss the main findings of the probabilistic assessment of the reference disposal system. In particular, we discuss

- *Estimated radiation doses to the critical group (Section 6.5.2)*. The mean ADE is calculated for times up to 10^5 a following disposal, and includes the ADEs from all 68 radionuclides (Table 5-4). Our analysis shows that the mean ADE for the reference disposal system meets the dose limit associated with the radiological risk criterion specified by the AECB (AECB 1987a). This limit is met even if the criterion were extended to 10^5 a after closure. Section E.2 in Appendix E shows that these conclusions are unchanged when considering recent revisions to the ICRP recommendations (ICRP 1991).

- *Chemical toxicity effects (Section 6.5.3)*. We calculate the arithmetic average of the estimated concentrations of nine chemically toxic contaminants (Table 5-3) in different parts of the biosphere.

  Our analysis indicates that these average concentrations are far below existing regulations or guidelines and are much smaller than naturally occurring concentrations in the biosphere. We conclude that these contaminants would have negligible adverse chemical toxicity effects.

- *Protection of the environment (Section 6.5.4)*. We examine the potential chemical and physical effects on the environment attributed to the presence of the disposal vault. The focus is on the arithmetic averages of estimated concentrations in different parts of the biosphere for all contaminants released from the disposal vault. We compare the estimated concentrations of a contaminant with its corresponding environmental increments to identify contaminants of concern. (An environmental increment is a measure of the variability of concentration of a contaminant in the natural environment.) We conclude that only ^{14}C and ^{129}I could exceed their environmental increments. However, no significant adverse effects are likely because estimated concentrations of both ^{14}C and ^{129}I are very small. In particular, estimated radiological effects on nonhuman biota would be insignificant.

- *Sensitivity analysis (Section 6.5.5)*. In Section 6.5.5 and Sections E.3 to E.6 in Appendix E we identify and examine the important parameters in the probabilistic analysis. The probabilistic sensitivity analysis complements the deterministic sensitivity analysis (Section 6.3.3 and Sections D.5 to D.8 in Appendix D) by providing additional information on the effects of parameter uncertainty on estimates of impact.

- *Derived constraints (Section 6.6)*. We examine once again potential derived constraints. This topic is also discussed in Section 6.2, but the analysis in Section 6.6 is extended to consider the effects of uncertainty and to examine the influence of assumed site and design features.

6.5.2 Radiological Effects

The radiological effect of most concern in this report is the annual effective dose equivalent, or "annual dose," to humans. It is the radiation dose attributed to the reference disposal system and accumulated within one year by a member of the critical group. It combines (Davis et al. 1993)

- effective dose equivalent resulting from external exposure, and
- 50-year committed effective dose equivalent resulting from the ingestion and inhalation of radioactive contaminants.

The estimates of annual dose discussed in this report are based on the 1977 recommendations of the ICRP (ICRP 1977, Davis et al. 1993). Section E.2 in Appendix E describes how the ADEs and radiological risk would be affected by the 1990 recommendations (ICRP 1991).

The ADE is the sum of the estimated annual doses from all 68 radionuclides of concern (listed in Table 5-4 and discussed in Section 5.9). It is a function of time and is calculated at selected times up to 10^5 a following vault closure. We also frequently qualify the ADE by referring to a specific radionuclide and time; for instance, the ADE at 10^4 a resulting from ^{129}I is the annual dose that is estimated for the radionuclide ^{129}I at 10^4 a following vault closure.

For comparison with radiological criteria, we calculate the arithmetic mean (AECB 1987a) of the ADE for a set of randomly selected simulations. It is referred to, henceforth, as the mean ADE. We may also qualify the mean ADE to refer to a specified radionuclide and time; for example, the mean ADE from ^{129}I at 10^5 a is the arithmetic mean of the ADEs attributed to ^{129}I at 10^5 a from a set of randomly selected simulations.

The mean ADE is calculated as follows.

- For each randomly sampled simulation, we calculate the ADEs as a function of time, using a sufficiently large number of points to produce a smooth dose-time curve. However, we save only 25 values of the ADE at 25 specified points in time to conserve computer storage space. Twenty-five values are saved for all 68 radionuclides.
- The same set of 25 specified points in time is used in all randomly selected simulations.

The saved results from the sets of simulations are then averaged to give the mean ADE at the 25 prespecified points in time. These 25 selected points in time range from the time of closure of the reference disposal vault to 10^5 a in the future. They are chosen to give acceptable plots of the mean ADE against time using linear or logarithmic time-scales.

Finally, we use terms such as maximum of the mean ADE up to 10^5 a. These maxima may be calculated in two different ways.

- If no radionuclide is specified, the "maximum of the mean ADE" is a maximum in the total dose for all 68 radionuclides. The value reported is equal to the maximum in the mean ADE at the 25 selected points in time. For the reference disposal system, this maximum always occurs at 10^5 a.

- If a radionuclide is specified, we calculate a different arithmetic average from a set of simulations. The saved results for each simulation include (in addition to the above 25 selected points) the maximum ADE observed for every radionuclide, and the time at which this ADE occurred. We call the average of these maxima ADEs the "maximum of the mean ADE resulting from ^{129}I" (for example). (We use this label because it is similar to the "maximum of the mean" discussed above. However, a more accurate label would be the "mean of the maximum ADE from ^{129}I." Note the maximum of the mean is less than or equal to the mean of the maxima).

Figure 6-17 shows the distribution of the ADEs at 10^4 a from a set of 40 000 randomly selected simulations involving the seven radionuclides ^{14}C, ^{135}Cs, ^{129}I, ^{59}Ni, ^{107}Pd, ^{79}Se and ^{99}Tc from used fuel. (The ADE at 10^4 a of all other radionuclides fall within the first interval of the histogram.) This distribution of ADEs results from the combined effects of the uncertainties of all the parameters (described by their PDFs) used in the system model. The two curves in Figure 6-17 show that most estimates of annual dose are very small; in fact 99.8% of the ADEs are less than 9×10^{-10} Sv/a. There are only a few simulations with larger annual dose estimates, up to a maximum of about 3.7×10^{-8} Sv/a.

This latter observation can be compared with the discussion in AECB Regulatory Document R-104 (AECB 1987a) that states "it is judged acceptable to allow 5% of the estimated doses to exceed a dose of 1 mSv per year to take account of normal statistical variations which are inherent in the probabilistic assessment process." The results in Figure 6-17 show that all ADEs are far smaller than 1 mSv/a.

The mean ADE at 10^4 a is 1.0×10^{-11} Sv/a and would fall within the first interval of the histogram in Figure 6-17. Figure 6-18 shows a curve of mean ADE versus time. The mean is summed over ADEs from the seven radionuclides ^{14}C, ^{135}Cs, ^{129}I, ^{59}Ni, ^{107}Pd, ^{79}Se and ^{99}Tc from used fuel. All other radionuclides listed in Table 5-4 (Section 5.9) do not make a significant contribution to the sum or to the mean ADE for times up to 10^5 a.

The dashed lines on either side of the mean ADE are the 95% confidence bounds on the curve. These confidence bounds (see Section A.3.5 of Appendix A) indicate the statistical degree of precision of the curve:

- bounds formed in this way, 95 times out of 100, are expected to enclose the "true" value of the mean at any specific time, where the "true" value is the mean that would be obtained from an infinitely large population of simulations. (We also believe that this "true" value would be greater than the value that would occur if the reference disposal system were a reality because we have introduced many conservative assumptions in constructing its system model.)

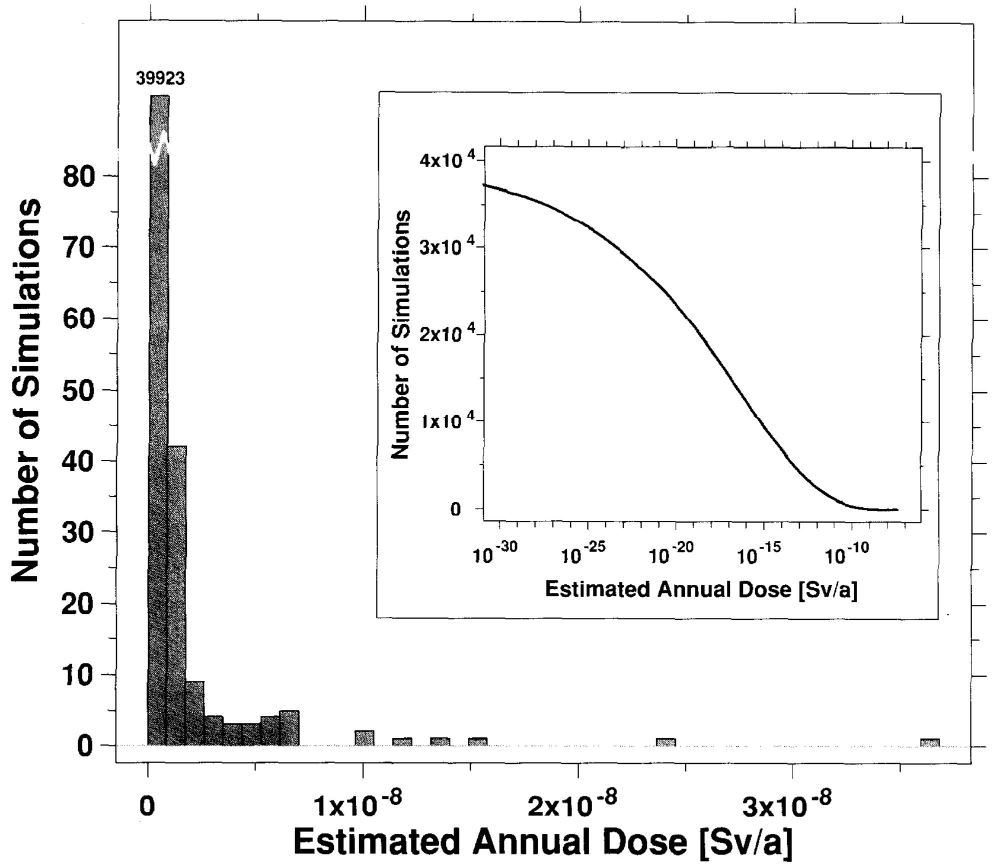

FIGURE 6-17: Distribution of Annual Dose Estimates at 10^4 a

These plots are based on results from 40 000 randomly selected simulations involving ^{14}C, ^{135}Cs, ^{129}I, ^{59}Ni, ^{107}Pd, ^{79}Se and ^{99}Tc from used fuel. (Results from all other radionuclides in Table 5-4 would fall within the first interval of the histogram.)

The horizontal axis for the histogram uses a linear scale to plot intervals for the annual dose estimate (ADE). The first interval ranges from 0.0 to about 0.9 x 10^{-9} Sv/a. The vertical axis shows the number of simulations having different ADEs. Note the break in the vertical axis and in the first interval; it makes the other intervals more visible. In fact, the height of the first interval should be more than 900 times larger than the second. The histogram shows a highly skewed distribution. A total of 39 923 simulations out of 40 000, or 99.8%, fall within the ADE range of the first interval, and 0.2% in all other intervals. There are only a few simulations with ADEs greater than 0.9 x 10^{-9} Sv/a, and the maximum observed value is 3.7 x 10^{-8} Sv/a.

The inset figure uses a logarithmic dose scale to illustrate better the wide range of ADEs. This complementary cumulative distribution function shows the number of simulations on the vertical axis that exceed a corresponding ADE given on the horizontal axis. It more clearly shows that only a very small fraction (about 0.1%) of the ADEs exceed 10^{-9} Sv/a, and the majority of the ADEs are much smaller than 10^{-15} Sv/a.

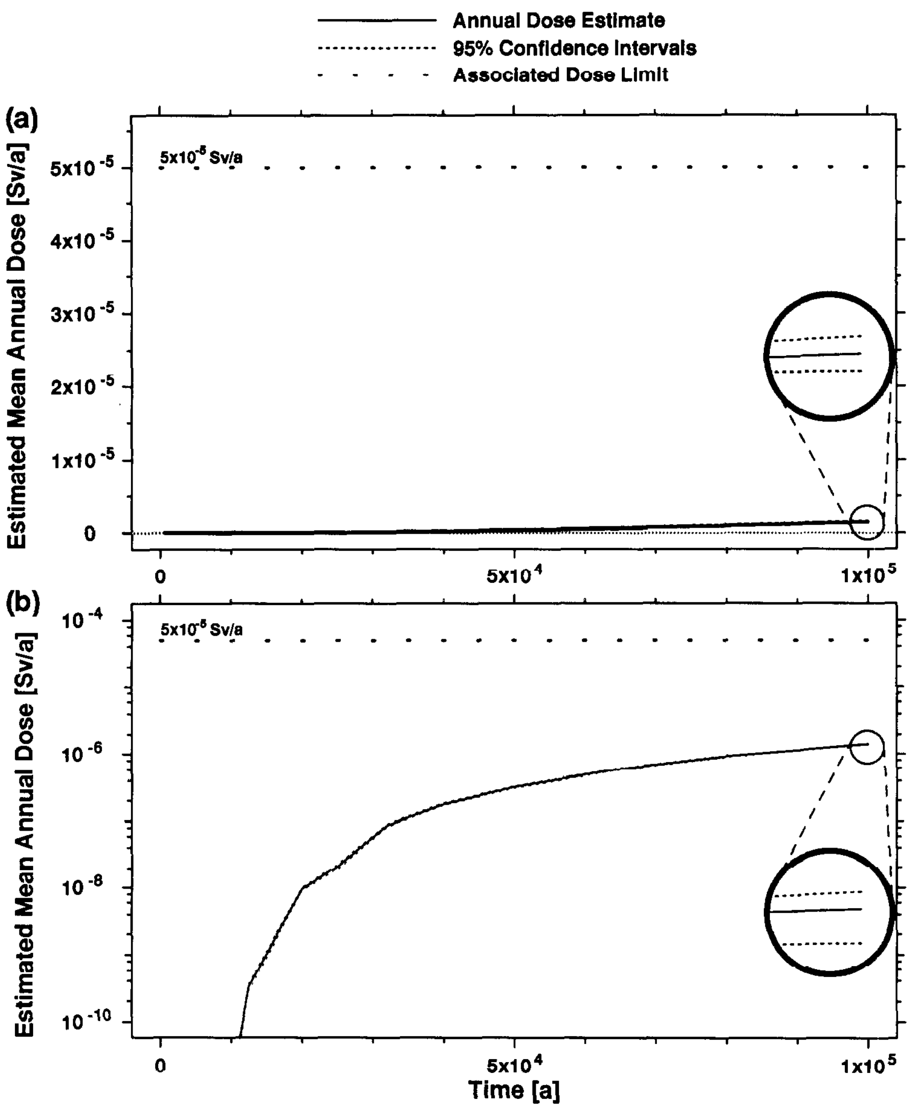

FIGURE 6-18: Variation of Mean Annual Dose Estimate with Time

These two plots show the same data but the vertical axes are linear in (a) and logarithmic in (b). In both plots, the horizontal line represents the annual dose of 5 x 10^{-5} Sv/a associated with the AECB radiological risk criterion (and prescribed for times up to 10^4 a) (AECB 1987a). The linear axis shows that estimated doses are very small but slowly increasing for times up to 10^5 a. (Results extended to longer time-scales show a maximum in the estimated dose curve near two million years.)
In each plot, the solid line shows the mean ADE. The dashed lines on either side of the mean ADE, illustrated more clearly in the circular insets, are the 95% confidence intervals based on statistical variation of the simulation results. At any particular time, the "true" value of the mean ADE would lie between the 95% confidence intervals 95 times out of 100, for the given models and data and the same number of simulations (Section A.3.5 in Appendix A). The "true" mean refers to the mean that would be obtained from an infinitely large number of simulations. The displayed confidence intervals suggest that the mean ADE has been determined relatively precisely.

Figure 6-18 also indicates for comparison the "associated" annual dose limit. The associated annual dose limit is the value of dose associated with the radiological risk criterion set by the AECB and has a value of 5×10^{-5} Sv/a (AECB 1987a). Its value is about 2% of the annual dose that residents of the Canadian Shield receive now from environmental sources of radiation.

From Figure 6-18, it is clear that the mean ADE is much less than the associated dose limit over the entire time of the simulations, 10^5 a. In particular, at 10^4 a the mean ADE is only 1.0×10^{-11} Sv/a, more than six million times smaller. It is smaller still at times before 10^4 a.

We can also calculate the conditional risk for the SYVAC scenarios, following the radiological risk equation defined by the AECB (AECB 1987a). At 10^4 a, it is equal to the product of 1.0×10^{-11} Sv/a and 2×10^{-2} fatal cancers and serious genetic effects per sievert (AECB 1987a), or about 2×10^{-13} fatal cancers and serious genetic effects per year. The conditional risk is thus more than six million times smaller than the risk limit. The risk limit itself is a small value, a probability of one in a million of a serious health effect per year (AECB 1987a).

Moreover, this risk applies to a small and select group of people. They are the members of the critical group whose characteristics are chosen such that they would be most at risk. The risk to an individual in any other group of people would be considerably smaller.

The estimated confidence bounds in Figure 6-18 provide strong evidence to support the conclusion that mean ADEs from the SYVAC3-CC3 model for the reference disposal system would meet the associated annual dose limit of 5×10^{-5} Sv/a for times up to 10^4 a, and even for times up to 10^5 a. Statistically, there remains a small possibility that large ADEs could be calculated using SYVAC3-CC3. As discussed in Appendix C, an annual dose at or above 1 Sv/a is in the nonstochastic range, where serious health effects are likely to occur (ICRP 1993). If these large-dose estimates are encountered with sufficient frequency, it is possible that the mean ADE could exceed the dose associated with the radiological risk criterion. However, we observe that

- No large annual doses are observed in any simulation performed with SYVAC3-CC3, including

  - 40 000 randomly sampled simulations performed for the seven radionuclides (^{14}C, ^{135}Cs, ^{129}I, ^{59}Ni, ^{107}Pd, ^{79}Se and ^{99}Tc from used fuel) expected to be the major contributors to dose;

  - 2000 randomly sampled simulations performed for all other radionuclides;

  - tens of thousands of simulations used for sensitivity analysis (including deterministic and probabilistic sensitivity analysis using extreme values for the fractional factorial designs);

  - tens of thousands of simulations using modified models and data to evaluate derived criteria; and

- a small set of simulations undertaken to search for the worst-case simulation.

  All observed annual doses are below 1 Sv/a at all times in all simulations. The largest observed ADE in the 40 000 randomly sampled simulations is about 3.7 x 10^{-8} Sv/a for times up to 10^4 a; it is shown as the single simulation on the large-dose side of Figure 6-17. For times up to 10^5 a, the largest ADE in the 40 000 simulations is about 2.9 x 10^{-4} Sv/a. These results suggest that serious health effects are extremely unlikely.

- With 40 000 simulations, we can estimate an upper limit of the probability that annual doses greater than 2.9 x 10^{-4} Sv/a might occur in subsequent results from SYVAC3-CC3. It is, with a 95% confidence bound, about 0.000075 (Andres 1986). That is, annual doses in excess of 2.9 x 10^{-4} Sv/a have a (statistical) probability of occurrence of less than one in 13 000 with a confidence bound of 95%, for the reference disposal system.

If the probability of occurrence of large annual doses (greater than 1 Sv/a) is less than one in a million, then it follows that they would not cause the conditional risk (based on the AECB risk equation) to exceed a risk limit of one in a million. We could demonstrate statistically that this is the case for the reference disposal system by conducting more simulations. In principle, to establish a risk of no more than one chance in a million of a serious health effect (at the 95% confidence level), more than three million simulations would be required (Andres 1986).

While we could perform and analyze three million simulations using available computers, we believe it is not necessary. The analysis of a large number of simulations is strictly a statistical requirement that does not take advantage of the information that is available on the nature of the system model of the reference disposal system. This information is detailed and extensive, including studies during the development and testing of the system model and studies for the deterministic and probabilistic sensitivity analyses. On the basis of all information now available, we believe that there is no feasible and realistic combination of parameter values for the reference disposal system that would give rise to a large annual dose for times up to 10^5 a.

We obtain more information on the expected behaviour of the reference disposal system by examining the results of all the randomly sampled simulations. For instance, SYVAC3-CC3 calculates and stores the ADEs for each simulated radionuclide, and we can use the results to identify the main contributors to the mean ADE. (This is a preliminary type of sensitivity analysis.) The results show that only two radionuclides, ^{129}I and ^{14}C, make significant contributions to the mean ADE in all randomly sampled simulations at any time up to 10^5 a. Moreover, ^{129}I is clearly the dominant contributor. (In Section 8.2.6, we note that recent data for ^{14}C would considerably reduce its contributions to the mean ADE.) A similar observation is described in Section 6.3, pertaining to the annual dose estimated for the median-value simulation.

We have confirmed the dominance of ^{129}I and ^{14}C through further examination of results. For example, we have examined the ADEs for all radionuclides in all randomly sampled simulations. We searched for instances where, at any of the 25 specified time points, the ADE for a radionuclide exceeds 1% of the total ADE resulting from ^{14}C and ^{129}I from used fuel. This occurred in a total of just four simulations. Of these, three simulations involved ^{14}C from Zircaloy and one involved ^{39}Ar from used fuel. The largest contribution was just 1.3% of the total dose, from ^{14}C (Zircaloy) in one of the four simulations. Finally, we also conducted a similar examination of the simulations performed for the design constraint sensitivity analysis and note that ^{99}Tc from used fuel occasionally has a large ADE (but only for some simulations described in Section 6.6 and Section E.8 in Appendix E, in which contaminant transport avoids the backfill from vault rooms located above and to the right of fracture zone LD1).

Figure 6-19 shows the mean ADEs resulting from ^{14}C and ^{129}I as a function of time. The mean ADE for a radionuclide is calculated by averaging values for all randomly sampled simulations involving that particular radionuclide. Contributions from only two nuclides are large enough to be visible in the plots. Table 6-7 provides additional information. It shows the maximum value, over 10^5 a, of the mean ADE. Iodine-129 from used fuel clearly has the largest maximum: its mean maximum ADE of 1.4×10^{-6} Sv/a occurs at 10^5 a. (Simulations using SYVAC3-CC3 extended to longer timescales that show estimated doses from ^{129}I would attain a global maximum near 2×10^6 a.) The next largest value is due to ^{14}C from used fuel: its mean maximum ADE is 1.4×10^{-8} Sv/a and occurs near 4×10^4 a. For any other radionuclide in Table 5-4 (Section 5.9), the maximum of its mean ADE is less than and, generally, much less than, 10^{-10} Sv/a. For instance, the third largest contributor to total dose is ^{14}C from Zircaloy, and the maximum of its mean ADE is 9×10^{-12} Sv/a.

These mean nuclide ADEs are extremely small in comparison with the dose limit associated with the radiological risk criterion even when considering the criterion at 10^5 a. The largest mean ADE, from ^{129}I, is less than about 1.4×10^{-6} Sv/a for all times up to 10^5 a. From the AECB risk equation (AECB 1987a), this value corresponds to a conditional risk of about one in forty million of a serious health effect for times up to 10^5 a (the risk at 10^4 a is about 2×10^{-13} serious health effects per year, and the risk at earlier times is even smaller). Serious health effects from natural background radiation would be more than 2000 times more likely. The ADEs and risks from all other nuclides are much smaller.

These studies confirm our conclusion that, for the disposal system studied in this postclosure assessment, ^{129}I and ^{14}C are the only significant contributors to the mean ADE for times up to 10^5 a. Similar conclusions were reached in earlier assessments; for instance, Wuschke et al. (1985) reported that, for times up to 10^5 a, the major contributor to maximum annual dose equivalent was ^{129}I, whereas ^{14}C was a minor contributor, and ^{99}Tc and all other radionuclides made very small or insignificant contributions.

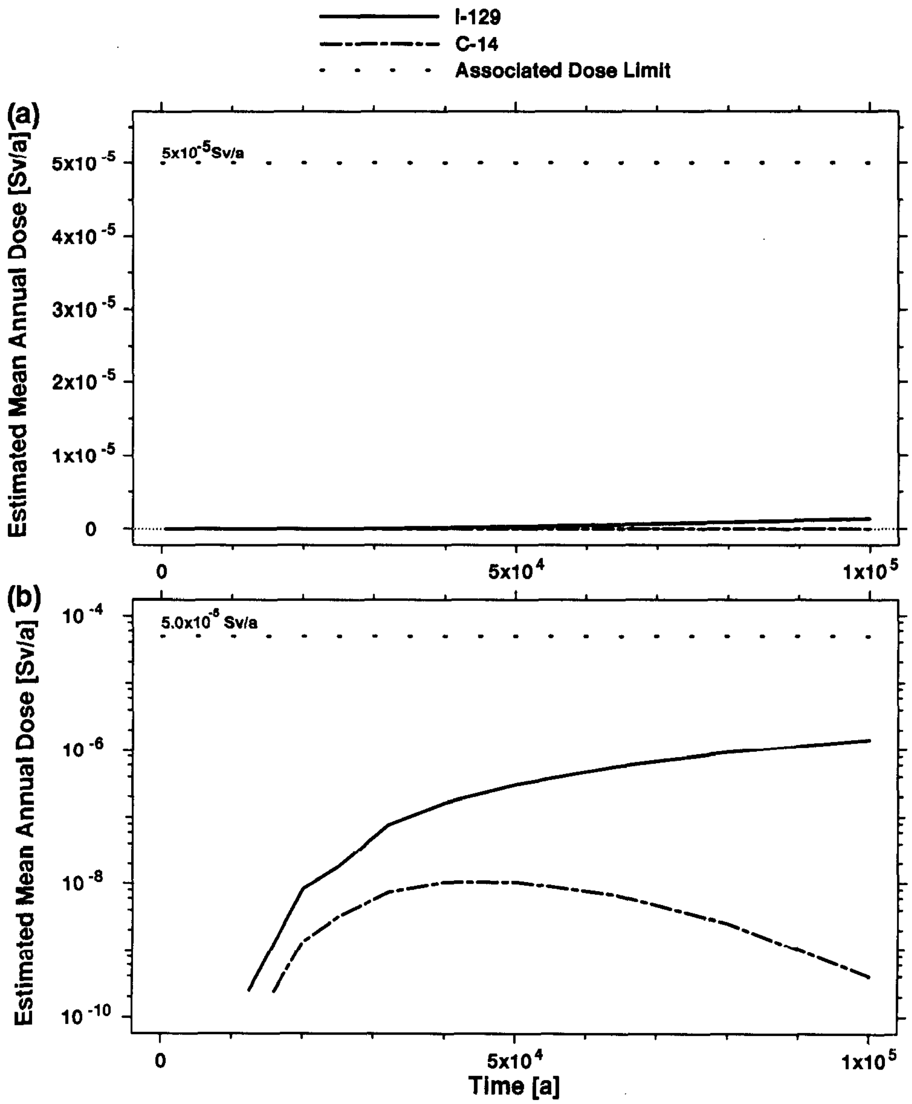

FIGURE 6-19: Variation with Time of Mean Annual Dose Estimate Attributed to Different Radionuclides.

Each curve shows the average, over 40 000 randomly sampled simulations, of the annual dose estimate (ADE) for the indicated radionuclide. Parts (a) and (b) show the same data but use different vertical axes. In both parts, the horizontal line represents the annual dose of 5 x 10^{-5} Sv/a associated with the AECB radiological risk criterion (AECB 1987a).

- For the linear vertical axis in part (a), only ADEs from ^{129}I are large enough to rise above the horizontal axis, and the effect is only obvious after about 5 x 10^4 a.
- The logarithmic vertical axis in part (b) exhibits a much wider range of estimated doses and shows curves for both ^{129}I and ^{14}C. The mean ADE from ^{14}C reaches a maximum near 4 x 10^4 a because radioactive decay is effective in reducing the amount of ^{14}C that could arrive at the biosphere at later times.

Although a total of 68 radionuclides (Table 5-4) is examined, only ^{14}C and ^{129}I from the used-fuel matrix are shown here because the ADEs from all other radionuclides are less (and generally much less) than 10^{-10} Sv/a for all times up to 10^5 a.

TABLE 6-7

MAXIMUM VALUE OF MEAN ANNUAL DOSE OVER 10^5 a

FOR DIFFERENT RADIONUCLIDES*

Radio-nuclide	Maximum up to 10^5 a of the Mean Annual Nuclide Dose (Sv/a)	Time of maximum (a)
^{129}I	1.4×10^{-6}	1×10^5
^{14}C	1.4×10^{-8}	4×10^4
All other nuclides listed in Table 5-4	$<1 \times 10^{-10}$	-

* Only two nuclides make significant contributions to mean annual dose estimate (ADE) over 10^5 a: ^{129}I and ^{14}C, both from the used-fuel matrix. The contribution from ^{129}I is several orders of magnitude greater than that from ^{14}C, which in turn has contributions many orders of magnitude greater than any other radionuclide. (More recent data for ^{14}C would lead to a significantly smaller contribution than that reported here whereas contributions from ^{36}Cl may be significant; see Section 8.2.6). Iodine-129 has a relatively long half-life (1.59×10^7 a), and its ADEs reach a maximum at 10^5 a (the time limit of the simulations) because of the slow movement of iodine from the vault to the biosphere. Carbon-14, with a much shorter half-life (5730 a), shows a peak ADE near 4×10^4 a because of its slow movement and radioactive decay. All other nuclides had mean ADEs that are many orders of magnitude smaller than 1×10^{-10} Sv/a, and most would have a time of maximum of 10^5 a. (Note the reported time of maximum cannot exceed 10^5 a because these simulations were performed only to 10^5 a.)

In light of the above observations, it is instructive to examine the characteristics of ^{129}I and ^{14}C to determine why their estimated radiation doses are dominant. We observe that these radionuclides have several important properties in common:

- Iodine-129 and ^{14}C both have relatively long half-lives (1.59×10^7 and 5730 a respectively). They are also mobile and are, therefore, transported relatively quickly (compared with contaminants that tend to sorb) from the vault to the biosphere. A significant fraction of their inventories are instantly released, and thus are available for transport at the instant of container failure (Johnson et al. 1994b). (Recent results indicate that the instant-release fraction for ^{14}C is 1 to 2 orders of magnitude smaller (Johnson et al. 1994b), so that its impacts reported in this postclosure assessment are greatly overestimated; see also Section 8.2.6) Finally, both radionuclides are relatively abundant in used fuel.

In contrast, we observe that

- Tritium (^3H) is instantly released and is mobile but it has a half-life of only 12.35 a. It virtually disappears because of radioactive decay before it could reach the biosphere.

- Cesium-135 has a relatively long half-life (2.3 x 10^6 a), and up to 25% of its inventory may be released from the used-fuel waste matrix at the instant of container failure (Johnson et al. 1994b). However, cesium is strongly sorbed onto the engineered barriers in the vault and onto many minerals in the surrounding rock. Thus ^{135}Cs is relatively immobile and does not reach the biosphere in appreciable quantities for times up to 10^5 a.

- Uranium-238 has a long half-life (4.5 x 10^9 a), but it is relatively immobile. As discussed in Section 6.3.3, most of the ^{238}U remains bound within the used-fuel matrix and any released ^{238}U is sorbed onto the buffer, backfill and rock surrounding the vault, for times up to 10^5 a.

- Krypton-81, a long-lived (2.1 x 10^5 a) radioactive isotope of a noble gas, is also instantly released from the used-fuel waste matrix and is mobile. Krypton-81, however, has a small inventory in used fuel. Moreover, the noble gases are not highly radiotoxic because they do not accumulate in biota. Radiation doses from ^{81}Kr (and ^{39}Ar and ^{85}Kr) would be caused almost entirely by external exposure, a much less significant exposure pathway than internal exposure.

Sensitivity analyses described in Section 6.5.5 provide more discussion on the important characteristics of ^{129}I and ^{14}C.

6.5.3 Chemical Toxicity Effects

In this section, we examine the potential harm to the critical group from nine chemically toxic contaminants in the used fuel and Zircaloy waste matrices: antimony, bromine, cadmium, cesium, chromium, molybdenum, samarium, selenium and technetium.

The magnitude of potential effects generally depends on contaminant concentrations in water, soil and air of the geosphere. The characteristics of the system model are such that the greatest concentrations of contaminants would be restricted to a small region of the biosphere in the vicinity of the critical group. This region includes the four discharge zones from the disposal vault (three to surface waters and wetlands with a small terrestrial component and the fourth to the well) and the garden, forage field, woodlot and peat bog used by the critical group.

The results indicate that estimated concentrations are very small in the biosphere for all simulations. Thus we have condensed the results by reporting only the mean values of the maximum concentrations that were estimated for times up to 10^5 a. That is, for each simulation, we first select the maximum concentration for a contaminant observed for times up to 10^5 a. We then calculate the arithmetic mean of these maximum concentrations.

Table 6-8 shows the results for garden soil, well water and indoor air (mean of maximum concentrations are smaller in the soils of other fields, in lake water and in outdoor air). Bromine has the greatest estimated concentrations: 3×10^{-9} mol/kg soil, 2×10^{-9} mol/m^3 water, and 2×10^{-16} mol/m^3 air. The next highest concentrations, for antimony, are orders of magnitude smaller. Estimated concentrations of the other seven chemically toxic elements are less than 10^{-20} (mol/kg of soil and mol/m^3 of air and water).

We conclude that there would be no measurable harm to the critical group from the estimated releases of bromine and antimony for several reasons.

- Their estimated concentrations are many orders of magnitude below existing environmental regulations. For example, limits on concentrations in water set by Health and Welfare Canada (1989) (see also McNeely et al. 1979) are approximately 10^{-3} mol/m^3 for bromine and 10^{-4} mol/m^3 for antimony.

- Their estimated concentrations are also far below concentrations of bromine and antimony normally found in the environment. For instance, Bowen (1979) cites median concentrations for bromine of 1×10^{-4} mol/kg soil and 2×10^{-4} mol/m^3 fresh water. Amiro (1992a) notes these same values are typical background concentrations of bromine in soil and water on the Canadian Shield. Thus median concentrations of bromine in the environment are 10^5 times or more greater than estimated mean concentrations for bromine from the disposal vault. For antimony, median concentrations are 1×10^{-5} mol/kg soil and 2×10^{-6} mol/m^3 fresh water (Bowen 1979) and background concentrations on the Canadian Shield are 2×10^{-6} mol/kg soil and 8×10^{-4} mol/m^3 water (Amiro 1992a). A soil cleanup level for antimony is 20 mg (2×10^{-4} mol)/kg soil (Government of Ontario 1989). Thus environmental concentrations of antimony are also many orders of magnitude greater than its estimated mean concentrations from the disposal vault.

- Their estimated concentrations in the environment would not lead to unacceptable ingestion levels. For example, a simple estimate of intake levels allows that members of the critical group drink two litres of water per day. If their drinking water was contaminated well water, their intake of bromine would be 3×10^{-10} g/day. We can then compare this estimated level of intake with toxicity intake data. Bowen (1979) reports a value of 3 g/day for bromine, or 10 orders of magnitude greater than the above estimate. Thus the ingestion of bromine attributed to the reference disposal vault would be far below toxic intake levels. Similar results are obtained for all other elements based on toxicity intake data from a number of sources. (One such source we examined is a risk assessment computer program (HRI 1993) whose data includes carcinogenic oral slope data and reference dose data from the U.S. Environmental Protection Agency databases "Integrated Risk Information System" and "Health Effects Assessment Summary Tables".)

TABLE 6-8

ESTIMATED CONCENTRATIONS* OF CHEMICALLY TOXIC CONTAMINANTS IN THE BIOSPHERE

Contaminant	Mean of the Maximum Estimated Concentration, Up to 10^5 a in		
	Garden Soil (mol/kg)	Well Water (mol/m^3)	Indoor Air (mol/m^3)
Antimony	2×10^{-18}	1×10^{-17}	$<10^{-20}$
Bromine	3×10^{-9}	2×10^{-9}	2×10^{-16}
Cadmium	$<10^{-20}$	$<10^{-20}$	$<10^{-20}$
Cesium	$<10^{-20}$	$<10^{-20}$	$<10^{-20}$
Chromium	$<10^{-20}$	$<10^{-20}$	$<10^{-20}$
Molybdenum	$<10^{-20}$	$<10^{-20}$	$<10^{-20}$
Samarium	$<10^{-20}$	$<10^{-20}$	$<10^{-20}$
Selenium	$<10^{-20}$	$<10^{-20}$	$<10^{-20}$
Technetium	$<10^{-20}$	$<10^{-20}$	$<10^{-20}$

* The above data are arithmetic averages, taken over all simulations, of maximum (to 10^5 a) estimated concentrations in garden soil, well water and indoor air. Only antimony and bromine have values exceeding 10^{-20}.

We also conclude that there would be no significant risk to the critical group attributed to the other seven chemically toxic elements. For six of these elements, mean concentrations are far below regulatory guidelines, where such guidelines exist, and far below typical concentrations that would be expected on the Canadian Shield. Their estimated intake levels are much smaller than their corresponding toxicity intake data.

The remaining element is technetium; it is of special interest because it does not have any stable isotopes. Its concentrations in the natural environment are extremely small: about 10^{-13} mol/kg in soil and 10^{-16} mol/m^3 in surface water (Amiro 1992a). (Bowen (1979) reports values as high as 10^{-13} mol/m^3 in rain water.) These values are much larger than the estimated concentrations of technetium. In addition, Coffey et al. (1984) suggest that the chemical toxicity hazard from technetium is similar to that of manganese. If this is the case, then the estimated concentrations for technetium would be far too small to cause any significant chemical toxicity effect.

We conclude that the chemically toxic elements from the disposal vault would not lead to significant chemical toxicity effects to members of the critical group. In fact, their estimated levels of contamination are so small that it would be impossible to infer the presence of a vault using the most sensitive of chemical and physical tests that are available today.

6.5.4 Protection of the Environment

In this section, we examine potential long-term impacts of the reference disposal system on the environment that result from the presence of the reference disposal vault. As discussed below, however, we expect that the effects would fall within existing (and assumed) environmental regulations and that the effects would be smaller than those now accepted for protection of the environment.

We first examine three potential postclosure impacts associated with construction of the reference disposal vault.

- *Impact of Excavated Rock.* The excavated rock produced during construction of the vault may be left exposed on the surface. This rock will be subjected to natural weathering processes and could release potential contaminants to the environment.

  The composition of the excavated rock would be similar to that of other rock and overburden exposed on the Canadian Shield. Thus the same types of contaminants would be released as are currently found on the Canadian Shield. An analysis of the short-term effects of this material is discussed in the primary reference for the preclosure assessment (Grondin et al. 1994), and it concludes that there would be no unacceptable toxic releases. A similar conclusion applies for times up to 10^4 a and longer, assuming the continued processes of slow, natural, weathering. (Note that the excavated rock should not be compared with tailings associated with the extraction of ores from mines because such ores are often found in association with significant quantities of reactive minerals, such as sulphides and arsenides.)

- *Impact of Residues from Explosives.* Groundwaters discharged to the biosphere may be enriched in nitrates from explosives used to excavate the vault.

  These materials will be discharged at a greater rate during the construction and operation stages, and their discharges would be closely monitored to ensure compliance with all environmental regulations. We believe that any potential effects after closure of the vault would be negligible because there would be no pumping of infiltrated water from the sealed vault and because natural discharges of water would be small once the vault has been backfilled and sealed.

- *Impact of Surface Temperature Rise.* The radioactive material in the reference disposal vault will continue to release energy for thousands of years and could elevate the temperature of the surface environment.

  Estimates of energy flows, including consideration of natural ground heat fluxes, indicate that the temperature rise at the surface, attributed to the disposal vault, would be much less than 1°C (Amiro 1992c). This very small temperature rise would have no significant effect on the environment.

We conclude that these potential long-term impacts are of no further concern for the postclosure assessment of the reference disposal system.

Other potential impacts are associated with the potential release of contaminants from the disposal vault. In the discussion that follows, we identify all the contaminants that might significantly increase typical background concentrations found on the Canadian Shield. We then draw some conclusions about the potential effects on the environment, including radiological effects on nonhuman biota.

6.5.4.1 Contaminants Reaching the Environment

We consider the 68 radionuclides and nine chemically toxic elements listed in Tables 5-3 and 5-4 (Section 5.9). The results of the probabilistic simulations show that their estimated concentrations in all the parts of the biosphere used by the critical group are extremely small. Therefore, we have summarized the results in the same manner as in Section 6.5.3, and we examine the mean values of the maximum estimated concentrations, where the maxima are over times up to 10^5 a following closure of the vault.

We assume that no further consideration is warranted for contaminants whose estimated concentrations are less than the extremely small values of 10^{-20} mol/kg dry soil and 10^{-20} mol/m^3 water or air. Table 6-9 summarizes the results and notes that only five contaminants have values greater than 10^{-20} (mol/kg dry soil or mol/m^3 water or air):

- Of the 68 radionuclides, ^{129}I has the largest estimated concentrations. The means of its maximum estimated concentrations are 2×10^{-9} mol/kg dry soil, 4×10^{-9} mol/m^3 water, and 5×10^{-14} mol/m^3 air. The estimated concentrations amount to less than one part per billion by weight in these media for all times up to 10^5 a.

- The radionuclide with the second largest estimated concentrations is ^{14}C from used fuel; its concentrations are at least 4 orders of magnitude smaller that those for ^{129}I. Concentrations of all other radionuclides are many orders of magnitude smaller that those for ^{129}I.

- Of the chemically toxic contaminants, bromine has the largest estimated concentrations. The means of its maximum estimated concentrations are 3×10^{-9} mol/kg dry soil, 2×10^{-9} mol/m^3 water, and 2×10^{-16} mol/m^3 air. The other chemically toxic contaminants have much smaller concentrations.

These estimated concentrations apply to the small region of the biosphere occupied by the critical group and other biota. To evaluate their potential to cause environmental impacts, we require established and quantitative regulations or other guidelines for protection of the environment. Such regulations and guidelines are not generally available. Thus we have assumed criteria we believe can be used in a rigorous and demanding test to identify contaminants that could have significant impacts. The criteria and test, outlined below, are documented in more detail by Amiro (1992a, 1993) and Davis et al. (1993).

TABLE 6-9

ESTIMATED CONCENTRATIONS AND ENVIRONMENTAL INCREMENTS FOR SOME CONTAMINANTS*

Contaminant	Medium	Mean of Maximum Estimated Concentration**	Environmental Increment***
Antimony	Soil	2×10^{-13} mg/kg	0.2 mg/kg
	Water	1×10^{-15} mg/L	1×10^{-3} mg/L
Bromine	Soil	2×10^{-4} mg/kg	2. mg/kg
	Water	2×10^{-7} mg/L	1×10^{-3} mg/L
	Air	2×10^{-16} mol/m^3	
^{14}C	Soil	9×10^{-3} Bq/kg	9×10^{-3} Bq/kg
	Water	5×10^{-4} Bq/L	2×10^{-5} Bq/L
	Air	1×10^{-5} Bq/m^3	
^{14}C Z	Soil	9×10^{-6} Bq/kg	9×10^{-3} Bq/kg
	Water	2×10^{-7} Bq/L	2×10^{-5} Bq/L
^{129}I	Soil	2×10^{0} Bq/kg	1×10^{-5} Bq/kg
	Water	3×10^{-3} Bq/L	4×10^{-8} Bq/L
	Air	4×10^{-5} Bq/m^3	

* Results have been examined for all the contaminants listed in Tables 5-3 and 5-4 (Section 5.9), but the estimated concentrations for all but the five listed are less than 10^{-20} mol/kg dry soil and 10^{-20} mol/m^3 air or water. Those listed are from the used-fuel matrix, except ^{14}C Z which is from the Zircaloy matrix.

** SYVAC3-CC3 calculates concentrations in units of mol/kg dry soil and mol/m^3 water or air. The concentrations reported here have been converted to the units required for comparison with environmental increments. The data shown are arithmetic averages of maximum (for times up to 10^5 a) estimated concentrations for the reference disposal system in garden soil, well water and indoor air used by the critical group and other biota. (Concentrations in other soils, in lake water and in outdoor air are smaller.) The means are calculated from a set of 9000 randomly sampled simulations for ^{129}I and ^{14}C and a set of 1000 simulations for all other contaminants.

*** Environmental increments (defined in the text) are for the soil and water compartments of the biosphere (Amiro 1993, 1992a). The environmental increments for ^{14}C depend on the stable carbon content in the environment (Amiro (1993). The values reported here use typical values for stable carbon in soil and water: 9.3 g stable carbon/kg dry soil (a conservative minimum value) and 15.1 mg stable carbon/L water (taken from McKee and Rowsell (1984)).

The assumed criteria involve background (or baseline) concentrations of radionuclides and chemically toxic elements that currently exist on the Canadian Shield. The test involves a comparison of these background concentrations with our estimated concentrations of radioactive and chemically toxic contaminants. We assume that a contaminant from the disposal facility would not harm the environment if its estimated concentration falls within a measure of the *variability* of its background concentration in the natural environment (Amiro 1992a, 1993; Amiro and Zach 1993). This measure of variability is referred to as the environmental increment:

> The Environmental Increment (EI) value is the additional amount of nuclide that can be added to the background level without exceeding the natural, local, spatial variation in concentration. This value is sufficiently stringent so that if the additional contribution from a vault is less than this, the presence of an underground vault would not likely cause detectable environmental effects (Amiro 1992a).

For example, concentrations of bromine in soils on the Canadian Shield typically vary between 5 and 40 mg/kg, with an average background concentration of about 10 mg/kg and a standard deviation of 2 mg/kg. On the basis of these data, we take its environmental increment to be 2 mg/kg (Amiro 1992a). Our estimated concentration of bromine is 2 x 10^{-4} mg/kg, or 4 orders of magnitude smaller. Similar observations apply to bromine concentrations in water. Thus we conclude that bromine associated with discharges from the reference disposal vault would have no detectable environmental impacts.

Table 6-9 includes environmental increments for the five contaminants of concern. (Environmental increment data for air are not available for most contaminants. We assume that the missing data would not affect our conclusions because estimated concentrations in air are linked to and proportionally smaller than estimated concentrations in soil and water). Comparison of the environmental increments with estimated concentrations shows that, for all 68 radionuclides and nine chemically toxic elements listed in Tables 5-3 and 5-4, only two contaminants exceed their environmental increments for soil or water (even when considering estimated concentrations that are less than 10^{-20} mol/kg dry soil or mol/m^3 water).

- Carbon-14 exceeds (or equals) its environmental increments for soil and for well water (but not for surface waters because estimated maximum concentrations in lake water are orders of magnitude smaller than estimated concentrations in well water). Most of the ^{14}C in the environment is produced naturally by cosmic ray interactions with atmospheric nitrogen.

- Iodine-129 also exceeds its environmental increments for both soil and water. This radionuclide exists in extremely small quantities in the environment, and it arises from reactions between cosmic rays and the atmosphere, from natural fission and from testing of nuclear weapons.

Because ^{14}C and ^{129}I exceed their environmental increments, we examine further their potential effects in soil and water. We evaluate both their chemical toxicity and their radiotoxicity effects in the following paragraphs. The next section presents a more detailed consideration of potential effects on nonhuman biota.

Chemical toxicity effects from ^{129}I are implausible because increased concentrations of ^{129}I from the disposal vault are negligible when compared to existing concentrations of iodine in the environment. Iodine (principally as the stable isotope ^{127}I) is relatively ubiquitous in the biosphere; Bowen (1979) cites a median concentration of 4 x 10^{-5} mol/kg dry soil, which is about 5 orders of magnitude greater than the maximum estimated concentration of ^{129}I in soil (Table 6-9).

Chemical toxicity effects from ^{14}C are not credible. Carbon is generally not regarded as a chemically toxic element; in fact, it is an essential nutrient required by all biota. Even if carbon were chemically toxic, it is already more abundant (as the stable isotope, ^{12}C) in the environment than it would ever be from the disposal vault.

Radiological effects attributed to ^{14}C and ^{129}I are also insignificant. Section 6.5.2 notes that the ADEs to an individual of the critical group from these two radionuclides are much smaller than the total annual dose arising from natural sources of radiation for all times up to 10^5 a. Although these estimated doses pertain to the critical group, we are not aware of any other biota that are likely to suffer significant adverse effects because of increased food-chain transfer or susceptibility to radiation from ^{14}C or ^{129}I (see, for example, ICRP (1977); Meyers (1989) and Zach et al. (1991)). We provide more support for this conclusion in the discussion in Section 6.5.4.2.

We, therefore, conclude that there would be no significant adverse effects on the environment from the small concentrations of ^{14}C and ^{129}I (and all other contaminants) potentially released from the disposal vault.

6.5.4.2 Radiological Effects on Nonhuman Biota

In this section, we consider in some detail estimates of the potential radiological effects on nonhuman biota. In radiation protection practice, it is generally accepted that protection of human individuals will implicitly protect populations of other species. However, we recognize that some organisms could be more exposed than humans because of their different habitat and behaviour.

We have performed an analysis for four generic target organisms (Section 5.6.2.8): a plant, a mammal, a bird and a fish (Amiro and Zach 1993). The characteristics, habitat and resource utilization of these organisms are defined to be representative of a wider range of organisms frequenting the Canadian Shield.

We consider only the effects of three radionuclides. The first two are ^{129}I and ^{14}C, the radionuclides with the largest estimated concentrations anywhere in the biosphere. We also consider ^{99}Tc. Although ^{99}Tc does not exceed its environmental increments for the reference disposal system, it has been identified as a potential contributor to dose in some sensitivity analysis studies (notably in those simulations in Section 6.6, where the backfill is not in the contaminant transport pathway). (Amiro (1992a) cites environmental increments of about 10^{-14} mol/kg in soil and 10^{-17} mol/m^3 in surface water for ^{99}Tc, arising from the testing of nuclear weapons and the nuclear fuel cycle.)

The results for the reference disposal system show that estimated annual doses to the target organisms are very small. Thus we have summarized the results as before and report the mean value of the maximum ADEs for times up to 10^5 a. That is, for each of 1000 simulations, we first select the maximum estimated dose for each target organism and radionuclide. We then calculate the arithmetic average of these maxima. Table 6-10 shows the mean value of the maximum ADE to the four target organisms. For each organism, the estimates are small, less than 10^{-4} Gy/a, over the entire simulation period of 10^5 a. For all simulations, ^{129}I consistently reaches its maximum dose at 1 x 10^5 a, whereas ^{14}C reaches its maximum at times as early as 3 x 10^4 a, and the time is slightly different for different pathways.

The estimates of the total annual dose from ^{14}C, ^{129}I and ^{99}Tc in Table 6-10 are evaluated further, to determine whether they would likely cause detrimental effects. A methodology to convert radiation dose to risk has not been developed to encompass a wide range of plants and animals (such a methodology exists thus far only for humans). Therefore, we evaluate the estimated effects in the context of a large number of scientific studies that have investigated the effects of radiation exposure on plants and animals.

We use data from studies of the effects of chronic irradiation. The most relevant scientific studies are those carried out in natural systems involving plant and animal populations on the Canadian Shield. Some observations of the effects of chronic irradiation are summarized in Table 6-11. Of these, a bird population studied by Zach and Mayoh (1986) appears to be one of the most sensitive populations. The results in Table 6-11 suggest that radiation doses of about 1 Gy/a can be tolerated by a wide range of organisms of the Canadian Shield.

Rose (1992) reviewed much of the scientific literature on the effects of ionizing radiation on nonhuman biota and concludes that a dose of 1 Gy/a causes some minor, subtle effects on several groups of plants and animals. An expert International Atomic Energy Agency committee (IAEA) believes that there is no convincing evidence in the scientific literature that dose rates less than about 0.4 Gy/a will harm plant or animal populations (IAEA 1992).

Plants and animals (and humans) thrive in radiation fields that have always existed in nature, and it is reasonable to assume that these natural background doses do not cause unacceptable environmental effects. Total dose from natural, external sources is typically about 7 x 10^{-4} Gy/a in Canada (Health and Welfare Canada 1986). Plants and animals, however, experience larger doses through processes such as root uptake, ingestion and inhalation of natural radionuclides. For example, total annual dose from natural sources for fish range up to 3 x 10^{-3} Gy/a (IAEA 1976).

TABLE 6-10

ESTIMATED MAXIMUM ANNUAL DOSE TO FOUR TARGET ORGANISMS*

Nuclide	Mean** of the Maximum Annual Doses (Gy/a) up to 10^5 a to			
	Plant	Fish	Mammal	Bird
^{14}C	2×10^{-7}	2×10^{-5}	5×10^{-7}	5×10^{-7}
^{129}I	4×10^{-6}	3×10^{-6}	1×10^{-5}	5×10^{-5}
^{99}Tc	2×10^{-15}	1×10^{-16}	1×10^{-16}	3×10^{-16}
Total	4×10^{-6}	2×10^{-5}	1×10^{-5}	5×10^{-5}

* The four organisms are chosen to have generic properties, and we assume they are located in the potentially most contaminated parts of the discharge areas for the reference disposal system. Pathways considered are those that contribute to the internal and external doses (but excluding inhalation).

** The values reported are based on 1000 randomly sampled simulations; the means are arithmetic averages of the maximum (to 10^5 a) estimated annual dose from each simulation. The units of annual dose are gray per year (Gy/a). (This unit differs from the unit of dose for humans, Sv/a, by a dimensionless radiation quality factor. This factor has a value of unity for ^{129}I, ^{14}C and ^{99}Tc.)

Table 6-12 summarizes the potential effects from various environmental dose rates delivered as chronic exposures over long time periods. Annual doses near 10 Gy/a have noticeable effects on some organisms; however, dose rates less than 10^{-3} Gy/a have not been associated with any detectable biological effects. It is unlikely that total background dose rates in the range 10^{-3} to 10^{-1} Gy/a will cause unacceptable effects. Therefore, we assume that protection of the environment from radiological effects will be assured if the estimated dose rates are below the lower range of background, or 10^{-3} Gy/a (Amiro and Zach 1993).

The estimates in Table 6-10 are clearly smaller than 10^{-3} Gy/a: the largest estimate is only 5% of this lower range of background does rates. Moreover, our estimates of doses to these four generic target organisms are based on many conservative assumptions (Davis et al. 1993). Therefore, we conclude that there would be no significant radiological effects to nonhuman biota.

6.5.5 Sensitivity Analysis of the Probabilistic Results

6.5.5.1 Description of the Method Used

In this section, we focus on sensitivity analysis of the results from the probabilistic assessment. The two objectives are

- to identify all important parameters for the system model, and

TABLE 6-11

EFFECTS OF CHRONIC RADIATION ON NONHUMAN BIOTA OF THE CANADIAN SHIELD

Absorbed Dose (Gy/a)	Effect
Less than 0.05	No effects on breeding tree swallows (Zach et al. 1993)
Greater than 0.7	No direct effects on the two bird species studied, but birds did not breed (Zach and Mayoh 1982)
Less than 0.9	No effect on trees, which are more sensitive than other plants (Amiro and Dugle 1985, Dugle 1986)
Less than 3.5	No effect on aquatic organisms (NRCC 1983)
5	No genetic effect and no detectable ecological stresses in meadow voles (Ross 1984, 1986; Mihok et al. 1985)
Less than 9	Effects on some tree species (Amiro and Dugle 1985), depressed growth of balsam fir, one of the most sensitive tree species (Dugle 1986)
Greater than 40	Decrease in forest canopy cover; many herbaceous plants thrived and some species experienced enhanced growth because of the elimination of competing species (Amiro and Dugle 1985)
350	Depressed hatching success and growth of tree swallow nestlings (Zach and Mayoh 1986)

- to describe and explain the effects of these parameters on key results of the model calculations.

The sensitivity analysis described in Section 6.3.3 and Sections D.5 to D.8 in Appendix D identifies important parameters and describes their effects, but it is focussed on studies of the median-value simulation. This deterministic sensitivity analysis is equivalent to determining a partial derivative of an output variable with respect to a single input parameter, and it permits the observation of many subtle effects and interactions and the illustration of these effects using simple plots. Similar subtle effects and interactions are generally not readily observed in sensitivity analysis of the probabilistic results because of the wide range of parameter values that contribute to the results.

The probabilistic sensitivity analysis is approximately equivalent to evaluating the average effect (and not a partial derivative) of changing one parameter when all the other parameters are simultaneously free to vary

TABLE 6-12

SUMMARY OF EFFECTS OF CHRONIC RADIATION DOSE RATES TO NONHUMAN BIOTA*

Dose Rate (Gy/a)	Range and Comments
10^{-6}	x
	x Significantly below background
10^{-5}	x dose rates; effects are unlikely
	x and not detectable
10^{-4}	x
	x
10^{-3}	xx
	x Range of natural background dose
10^{-2}	x rates to a wide variety of plants
	x and animals
10^{-1}	xx
	x
10^{0}	x Potential subtle, chronic effects
	xx
10^{1}	x Some organisms affected; effects
	x increase with increasing dose rate
10^{2}	x

* These data summarize our conclusions on potential consequences from various dose rates to plants and animals, delivered as chronic exposures over long time periods. The data indicate no detectable effects occur to nonhuman biota in the environment at dose rates less than 10^{-3} Gy/a.

across their entire ranges of possible values. We use scatter plots to display the results, but the effects of many parameters can only be observed through statistical analysis of the data.

Many different objective functions can be evaluated in the probabilistic sensitivity analysis, such as the ADEs at some point in time, maximum ADEs to 10^4 or 10^5 a, estimated concentrations of radionuclides in the food chain, ADEs to nonhuman biota, and concentrations of chemically toxic elements in water, soil and air. As in Section 6.3.3, we focus the probabilistic sensitivity analysis on the maximum, for times up to 10^5 a, of the total ADEs and the ADEs from ^{14}C and ^{129}I to individuals in the critical group. We also examine the arithmetic average or mean values of these ADEs. Section E.3 in Appendix E discusses why these particular objective functions were chosen. There are two major reasons.

- Radiation doses to the critical group are important impacts, with doses being attributed to ^{14}C and ^{129}I for times up to 10^5 a (Section 6.5.2).

- It is conservative to choose the longer period, in the sense that maximum ADEs observed for times up to 10^5 a are greater (and cannot be smaller) than maximum ADEs up to 10^4 a. Moreover, the analyses using the longer time period tend to identify parameters that are important in attenuating ADEs, rather than important in merely delaying the arrival of contaminants in the biosphere.

Section E.3 in Appendix E also defines and uses several other objective functions. However, as used in this section, an important parameter is defined to be one that has a notable effect on either of two calculated parameters: the maximum ADEs from simulations that consider the full range of values for a single parameter, or the arithmetic average of the maximum ADEs from many simulations that consider the full range of values for all parameters. An important parameter may affect the magnitude or an ADE, or both the magnitude and the variability of the arithmetic average of the maximum ADEs.

The above definition of an "important" parameter precludes identification of any parameter that is not described using a PDF. In Section 6.3.3, we noted that the ADE from the median-value simulation is sensitive to variations in waste exclusion distance. However, our analysis assumes that the waste exclusion distance is fixed at a value of about 50 m and, therefore, the waste exclusion distance cannot be identified as an important parameter. Nonetheless the screening does show that the two most important parameters both refer to properties of the rock and water within the waste exclusion distance. We include in Section 6.6 a special probabilistic analysis of the effects of different waste exclusion distances.

Section E.3 in Appendix E details the method used for probabilistic sensitivity analyses. Iterated fractional factorial analysis (Section A.4.3.1 in Appendix A) is the major tool in the screening, although other sources of information also play a role. Some information comes from the deterministic sensitivity analysis (Section 6.3.3 and Sections D.5 to D.8 in Appendix D). A second important source is expert judgment; members of the Model Working Groups contributed to the screening described here by examining and confirming that the results obtained were consistent with their understanding, and they also performed independent sensitivity analyses on the vault model (Johnson et al. 1994b), the geosphere model (Davison et al. 1994b) and the biosphere model (Davis et al. 1993).

Section 6.5.5.2 summarizes the results of the screening to identify important parameters. For each of these parameters, we proceeded with investigations to show how and why they influence the results. Section 6.5.5.3 shows the effects of the two most important parameters; further analysis is provided in Sections E.4 to E.6 in Appendix E for many other parameters (including others identified using different objective functions).

Section E.7 in Appendix E describes a special study of the most important parameter, the tortuosity of the lower rock zone, to show how sensitivity analysis can help guide further research and data acquisition activities. The detailed analysis examines two effects: how changes in the values of tortuosity affect the magnitude of the estimated impacts and how changes to its uncertainty (or range of permitted values) affect the uncertainty in the estimated impacts.

This special study is of most value for parameters that are reducible (Hofer and Hoffman (1987) use the term Type 2 uncertainty). A *reducible* parameter is one whose uncertainty stems from a lack of knowledge, and this lack could, in principle, be reduced through further research. For an irreducible parameter, further research would not reduce its uncertainty, as might occur if uncertainty is dominated by inherent spatial and temporal variability. (In fact, the uncertainty in most parameters is a mixture of both reducible and irreducible components.) Expert opinion would be used to determine whether it is feasible to perform such research, and detailed sensitivity analysis would be used to determine how worthwhile the effort would be.

6.5.5.2 Summary of the Results of the Screening Process

The screening method used, iterated fractional factorial analysis, is similar to that used for the deterministic sensitivity analysis (Section 6.3.3 and Section D.5 in Appendix D), except that the selection of a parameter value is not restricted to values near its median. Instead parameter values are chosen from the 0.01, 0.5 or 0.99 quantiles of their PDFs (and values are chosen for switches to sample all important options). This choice permits examination of the effects of each parameter over its range of possible values and allows direct comparison of the effects of parameters that have different physical units and different PDFs.

Table 6-13 lists the eight system model parameters determined to be most important for the reference disposal system. There are many similarities and a few differences between the screening of probabilistic results and the corresponding screening for the deterministic results (Section 6.3.3).

- Six of the eight parameters in Table 6-13 also appear in Tables 6-3 and 6-4. They are the tortuosity of the lower rock zone, the groundwater velocity scaling factor, the free-water diffusion coefficient for iodine, the switch describing the source of domestic water, the buffer anion correlation parameter and the depth of the well.

- Two parameters in Table 6-13 are not identified as important for their effects on ADEs in the median-value simulation: the thickness of compacted lake sediment at Boggy Creek South and the retardation factor of iodine in compacted organic lake sediment. These two parameters have weak effects in the median-value simulation because both are associated with the lake pathway and the lake pathway is relatively unimportant when the well is the source of domestic and irrigation water for the critical group. In the probabilistic sensitivity analysis, the well is not always present, and thus pathways involving the lake would be more important.

TABLE 6-13

IMPORTANT PARAMETERS FOR THE PROBABILISTIC SIMULATIONS

Parameter*	Relative Importance**	Correlation Coefficient**
Tortuosity of the lower rock zone	-2000	-0.55
Groundwater velocity scaling factor	49	0.12
Retardation factor of iodine in compacted organic lake sediment	-15	-0.05
Free-water diffusion coefficient for iodine	14	0.13
Switch: source of domestic water (well or lake)***	9	0.51
Buffer anion correlation parameter	7	0.18
Thickness of compacted lake sediment at Boggy Creek South	-8	0.07
Depth of the well	2	0.06

* The parameters listed have the greatest effect on the maximum estimated annual dose for times up to 10^5 a. (This analysis actually considers just ^{129}I, ^{14}C and five other radionuclides. Other results have shown that only ^{129}I and ^{14}C make significant contributions to the maximum ADEs for times up to 10^5 a, taking into consideration all of the 68 radionuclides in Table 5-4.)

** The "relative importance" results are calculated using data from 512 simulations, in which each parameter takes on values corresponding to its 0.01, 0.5 or 0.99 quantiles. The reported results are the ratio of geometric means of the estimates of maximum ADEs from these 512 simulations: the geometric mean from simulations using 0.99 quantile values is divided by the geometric mean of simulations using 0.01 quantile values. If the ratio is less than unity, its negative reciprocal is taken. A positive ratio indicates that the maximum ADEs tend to increase as the parameter values increase. A negative ratio indicates that the opposite pattern (and that the negative reciprocal has been taken).
The "correlation coefficient" results, calculated from 1000 randomly sampled simulations, use the logarithms of the maximum ADEs and parameter values. Correlation coefficients vary between +1 and -1. A value of +1 (-1) means the logarithm of the maximum ADE is linearly dependent on the logarithm of the parameter and increases (decreases) as the parameter value increases. A correlation coefficient equal to zero implies that there is no apparent linear relationship between the maximum ADE and the parameter.

*** For this switch parameter annual dose estimates are generally greater when the well is the source of domestic water.

Definitions for some of these parameters follow.

- Tortuosity in rock is a measure of the effective increased transport distance for diffusion because of the winding nature of the interconnected aqueous pathway within the rock (Davison et al. 1994b).

- The groundwater velocity scaling factor is a dimensionless multiplicative factor used to describe the uncertainty in groundwater velocities in the geosphere (Davison et al. 1994b).

- The switch describing the source of domestic water determines whether domestic water comes from the well or from the lake.

- The buffer anion correlation parameter correlates values of the diffusion coefficient and capacity factors in the buffer for anionic species (Johnson et al. 1994b).

The most notable result from Table 6-13, and in accord with results discussed in Section 6.3.3, is the magnitude of the relative importance of the tortuosity of the lower rock zone: it is by far the most important parameter.

The list of influential parameters could be extended further. However, it becomes progressively more difficult to observe, both visually and statistically, the effect of a parameter as its relative importance declines. Hence we refer to the eight parameters in Table 6-13 as the "important" parameters; they have the largest influences on the maximum ADEs to individuals in the critical group.

Nonetheless, we also examine the effects of another 18 parameters in Section E.3, Appendix E. They were selected because expert opinion suggested they may be important or because they have notable effects on objective functions that isolate effects of the vault, geosphere and biosphere models (Section E.3, Appendix E). We refer to these 18 parameters in the discussion below as the less important parameters because they warrant further study even though their effects on the maximum ADEs are relatively small. We also refer to the remaining parameters as the unimportant parameters. (There are about 1400 sampled parameters in simulations involving ten nuclides (Section A.3.3, Appendix A). The analysis described here considers seven radionuclides and uses just over 1300 sampled parameters in the system model of the reference disposal system. Thus there are about 1300 unimportant parameters.)

The influences of parameters are confirmed by an analysis of sets of 500 simulations in which different combinations of important, less important and unimportant parameters are randomly sampled. (Section E.3, Appendix E describes further this regression analysis.) The analysis calculates R^2, or the coefficient of determination (Section A.4, Appendix A), based on the logarithms of the maximum ADEs to 10^4 and 10^5 a. The greatest possible value of R^2, unity, occurs when the examined set of parameters accounts for (or explains) all the variability in the maximum ADEs. Its smallest possible value, zero, occurs when the set of parameters explains none of the variability. The results are summarized in Table 6-14, and show that

TABLE 6-14

REGRESSION ANALYSIS ON PARAMETERS OF THE SYSTEM MODEL*

Simulation Set	Parameter Values: 8 Important Parameters	18 Less Important Parameters	1300 Unimportant Parameters	Coefficient of Determination (R^2)** to 10^4 a	10^5 a
1	random	random	random	1.00	1.00
3	random***	random***	median	0.86	0.83
5	random***	median	median	0.84	0.67
2	median	median	random***	0.04	0.03
4	median	random***	random***	0.04	0.07

* These results show the effects of the eight important parameters (Table 6-13) compared with 18 less important parameters (Table E-1 in Appendix E) and approximately 1300 other unimportant parameters. The columns labelled "parameter values" give the sampling strategies used with five sets of 500 simulations. The results show that a large fraction of the variability in maximum ADEs is attributed to the eight most important parameters. The 18 less important parameters explain some of the variability, and the 1300 unimportant parameters explain very little.

** The last two columns report the coefficients of determination (R^2) from a linear regression on the logarithms of the maximum ADEs to 10^4 or 10^5 a. Coefficients of determination are calculated using logarithms of the maximum ADEs (to 10^4 and to 10^5 a) for the seven radionuclides contributing most to radiation dose (notably ^{14}C and ^{129}I). The calculations use the maximum ADEs from simulation set 1 and the maximum ADEs from each of the other indicated simulation sets.

*** These parameters use the identical sequence of randomly selected values as is used in simulation set 1.

- The eight important parameters are more successful at explaining the maximum ADEs up to 10^4 a than up to 10^5 a. For example, R^2 for set 5 in Table 6-14 is 0.84 at 10^4 a and decreases to 0.67 at 10^5 a.)

- Taken together, the eight important and 18 less important parameters successfully explain the maximum ADEs at both 10^4 and 10^5 a. For example, R^2 for set 3 in Table 6-14 is 0.86 at 10^4 a and has decreased only slightly, to 0.83, at 10^5 a.

In other words, more than 80% of the variability in the estimates of maximum annual dose can be attributed to the cumulative variability of just the eight important parameters at 10^4 a and to the cumulative variability in the eight important and 18 less important parameters at 10^5 a.

The differing behaviour in variability at the two times can be explained from consideration of the shape of the dose-time curve for ^{129}I, which contributes most to the total ADEs. The curve in Figure 6-19 rises continuously over the entire time period in all simulations, but it becomes less steep with time. (If the simulations were extended further in time, the dose curve for ^{129}I would reach a global maximum at times beyond 10^6 a.) From these observations, we conclude that

- The maximum ADEs up to 10^4 a occur at the steeply rising part of the dose-time curve. Factors that can move this rising edge forward or back in time will have a strong influence on the maxima. We should, therefore, expect to identify parameters that are important because they can affect how long it takes ^{129}I to travel from the vault to the biosphere.

  In fact, the first four parameters in Table 6-13 are related to water movement and contaminant transport: the tortuosity is a measure of the increased distance for diffusive transport from the vault to fracture zone LD1, the groundwater velocity scaling factor affects how fast the groundwater moves, the retardation factor of iodine in compacted organic lake sediment describes how long the sediment can hold up ^{129}I, and the free-water diffusion coefficient for iodine determines how rapidly ^{129}I can move by diffusion.

- At longer times, the maximum ADEs will become less dependent on parameters that delay iodine transport and become more dependent on parameters that affect the magnitude of the maximum. This may already occur by 10^5 a as suggested by the reduced effect of the eight most important parameters. On the other hand, many of the 18 less important parameters affect the maximum of the ADEs that could be reached. (Section E.3 and E.4 in Appendix E discuss two examples: the maximum of the ADEs from ^{129}I are directly proportional to its initial inventory and instant-release fraction).

In considering the longer time frame of 10^5 a, we observe a shift in importance from the eight most important parameters to the 18 less important parameters. This observation supports our choice of maximum ADEs to 10^5 a to screen for important parameters, instead of maximum ADEs to 10^4 a. As noted earlier, this latter choice of the model response will tend to identify parameters that affect attenuation of impacts, rather than merely delay impacts.

Regression analysis shows that the eight important parameters affect the maximum ADEs. Figure 6-20 shows they also affect both the magnitude and the associated variability of the mean maximum ADE. Comparison of the curves in the figure shows that the widest confidence bounds and the largest estimates of annual dose occur when all parameters are randomly sampled. The confidence bounds are significantly narrower when the eight most important parameters are fixed at their median values.

Section E.3 in Appendix E contains further discussion on the identification of important parameters, including studies that confirm the completeness of Table 6-13.

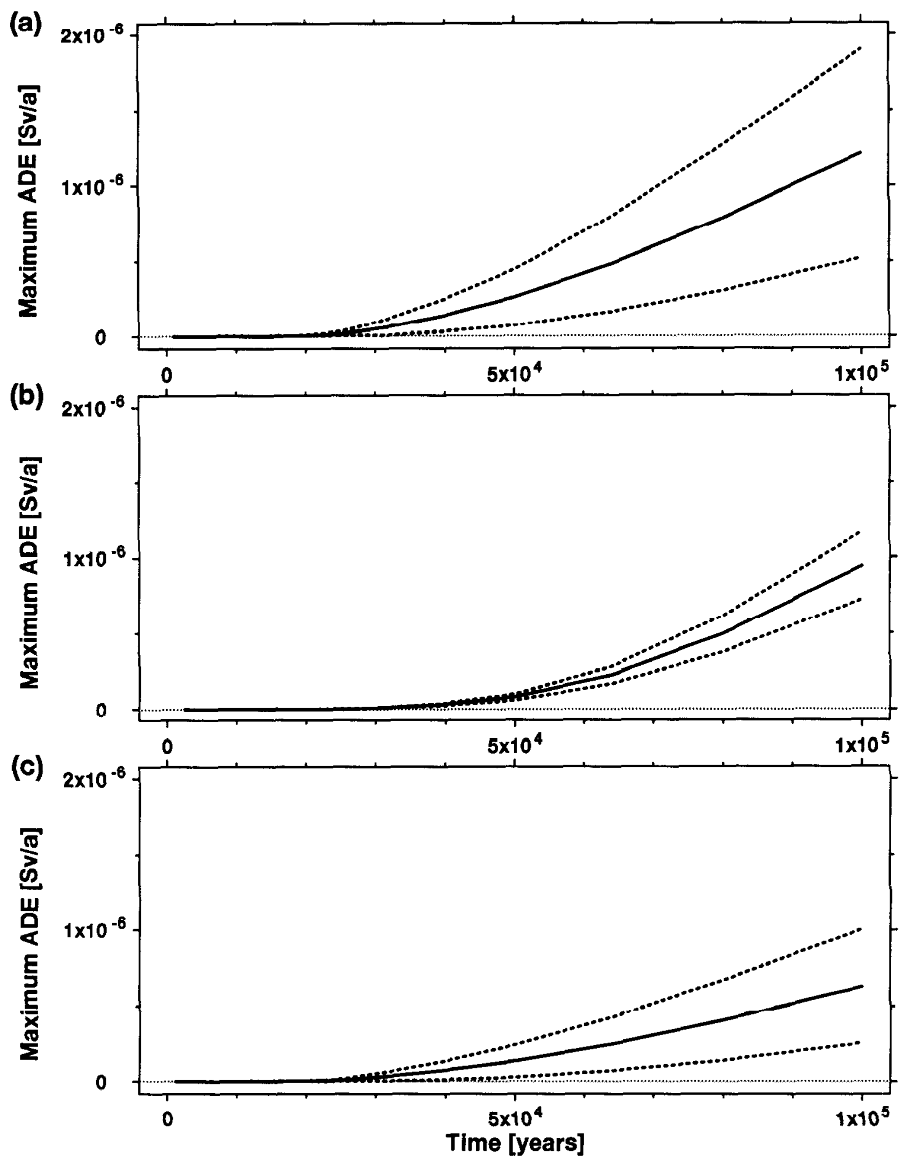

FIGURE 6-20: Mean Annual Dose Estimate Versus Time Showing the Effects of the Eight Important Parameters

These three plots show how the eight most important parameters affect the magnitude and variability in the mean annual dose estimates. In each plot, the horizontal axis is time, and the vertical axis is the mean annual dose estimate from 500 simulations. The dotted lines show the associated 95% Chebyshev confidence bounds (Section A.3.5 of Appendix A).

- Plot (a) shows results from set 1 (Table 6-14) in which all parameters are randomly sampled. (A similar curve shown in in Figure 6-18 is based on a much larger number of simulations.)
- Plot (b) shows results from set 4, where the eight most important parameters are fixed at their median value and all other parameters (more than 1300) are randomly sampled.
- Plot (c) shows results from set 5, where only the eight most important parameters are randomly sampled.

The detailed analysis in the following section considers three of the eight most important parameters. Sections E.4 to E.6 in Appendix E provide more detailed analyses for all of the eight important and 18 less important parameters.

6.5.5.3 Effects of Selected Important Parameters

We outline here the effects of three parameters that have a strong influence on the estimates of annual dose:

- the tortuosity of the lower rock zone,
- the groundwater velocity scaling factor, and
- the switch parameters that select the source of domestic water used by members of the critical group.

The first two parameters are clearly the most important in Table 6-13. They both describe properties of the rock and water in the waste exclusion distance and in other parts of the geosphere. Put another way, the uncertainty in estimates of annual dose are most strongly influenced by the uncertainties in two parameters that characterize the waste exclusion distance.

The switch parameter defines the use of well water or lake water and can be regarded as a parameter that selects between one of two mutually exclusive scenarios (Section 2.1 and Chapter 4).

Sections E.4 to E.6 in Appendix E provide more detail and discuss the effects of the other important parameters (as well as some additional parameters identified in Section E.3 of Appendix E that are important for their effects when considering different objective functions).

Tortuosity of the Lower Rock Zone

The tortuosity of the lower rock zone describes the increased effective distance for transport by diffusion resulting from the winding nature of the interconnected aqueous pathway (and does not pertain to transport by moving groundwater) (Davison et al. 1994b). It applies to all segments in the geosphere model, but takes on different values for segments in different zones of rock. Uncertainty in the tortuosity of the lower rock zone is the greatest source of variability in the maximum ADEs to 10^4 and to 10^5 a.

Figure 6-21 shows two scatter plots of the maximum ADEs to 10^4 and 10^5 a versus the tortuosity. (Sections E.4 and E.5 of Appendix E show similar plots for maximum ADEs from ^{129}I and ^{14}C.) The figure shows that the variation of the tortuosity causes a large variation in the magnitude of the maximum ADEs. There is more variability at 10^4 a than at 10^5 a. That is, uncertainty in the tortuosity of the lower rock zone results in more variability in the ADEs at early times than at later times, because tortuosity is primarily effective in delaying the movement of contaminants. At 10^4 a, mobile contaminants such as ^{129}I are just beginning to discharge at the biosphere in many simulations, whereas at 10^5 a the discharges are changing less quickly as a function of time for all simulations.

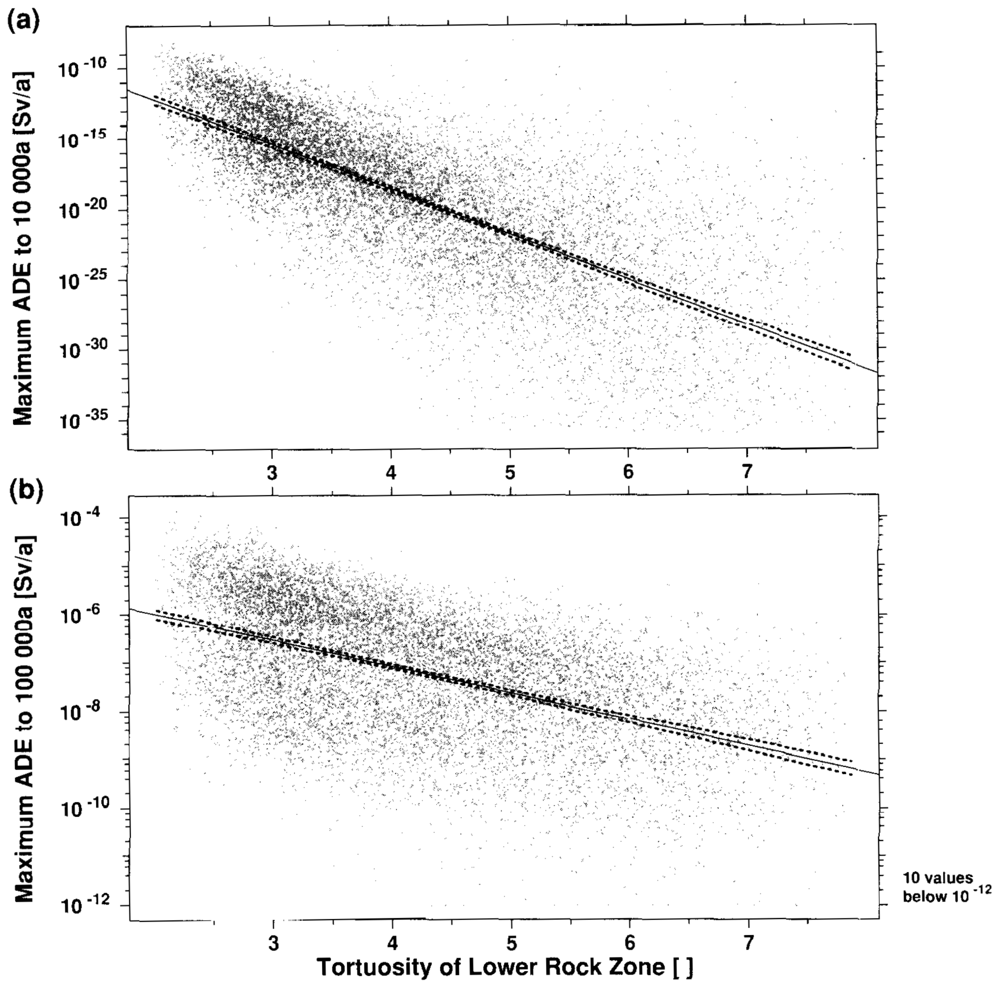

FIGURE 6-21: Effect of the Tortuosity of the Lower Rock Zone on Maximum Annual Dose Estimates

The vertical axes show the maximum ADEs from 10 000 randomly sampled simulations, where the maxima up to 10^4 a are shown in (a) and the maxima up to 10^5 a in (b). (We plot all calculated ADEs to display the range of estimates, even though the small values in part (a) may not be meaningful.) The horizontal axes show the tortuosity of the lower rock zone. Each plot also shows a trend line and the associated 95% confidence bands (Section A.4.3.3 in Appendix A); the trend line is the straight line obtained by performing a least-squares fit to the logarithms of the data. The correlation coefficients for the trend lines are -0.73 in (a) and -0.55 in (b).

These plots confirm that the tortuosity of the lower rock zone has a strong influence on maximum ADEs: larger values of tortuosity generally yield smaller ADEs, and uncertainty in the tortuosity leads to a large variability in the ADEs.

The trend lines indicate that the maximum ADEs tend to decrease as the tortuosity increases, in full accord with the sensitivity analysis of the median-value simulation (Section 6.3.3 and Sections D.5 to D.8 of Appendix D). These analyses have shown that the tortuosity of the lower rock zone is important because it has a strong influence on the rates of transport of contaminants by diffusion, especially at early times. It controls the transport of contaminants across the diffusion barrier of the lower rock zone, including rock within the waste exclusion distance that isolates the vault rooms from fracture zone LD1 (Section D.7.6 in Appendix D), and it also affects the rate of release of contaminants from the vault (Section D.6.4 in Appendix D). Similar conclusions are expected to apply to each simulation represented in Figure 6-21.

The figure demonstrates that the uncertainty in the tortuosity has strong effects on the maximum ADEs. The distribution of values for this parameter reflects the uncertainty in characterizing the diffusion properties of the lower rock zone. The PDF for tortuosity specified for SYVAC3-CC3 reflects a wide range of values obtained for a number of different rock types, and includes rocks from various locations on the Canadian Shield (Davison et al. 1994b).

It is possible that this distribution of values could be narrowed and its median shifted to larger or smaller values, once the host rock surrounding the vault has been more precisely characterized. These changes could reduce some of the variability in estimated impacts and increase or decrease the magnitude of the estimated impacts. Section E.7 in Appendix E investigates how possible changes to the PDF for the tortuosity of the lower rock zone would affect estimates of annual dose.

Groundwater Velocity Scaling Factor

The groundwater velocity scaling factor is applied uniformly to the entire network of segments simulated in the geosphere model (Section 5.4), and reflects the uncertainty in our knowledge of the groundwater flow system for the disposal system studied in this assessment over the time period of the simulations (Davison et al. 1994b).

Figure 6-22 shows two scatter plots of the maximum ADEs to 10^4 and 10^5 a versus the groundwater velocity scaling factor. (Sections E.4 and E.5 in Appendix E show similar plots for maximum ADEs resulting from ^{129}I and ^{14}C.) The figure shows

- the maximum ADEs tend to increase with larger values of the groundwater velocity scaling factor,

- the variability in the maximum ADEs is much greater at 10^4 a than at 10^5 a, and

- the effects of the groundwater velocity scaling factor are less important than the effects of the tortuosity of the lower rock zone (comparing Figures 6-21 and 6-22).

The detailed analysis of the median-value simulation (Section D.7.3 in Appendix D) shows that the groundwater velocity scaling factor influences the groundwater flow toward a bedrock well that intersects fracture zone LD1, the amount of diluting water drawn into the well, the fraction of contaminants moving in fracture zone LD1 that is captured by the well, the release of contaminants from the vault, and the transport in moving groundwater of contaminants in all segments. The complex effects described in Section D.7.3 of Appendix D should have a similar pattern in most of the simulations in Figure 6-22. The trend lines in this figure indicate the net effect, which is that smaller values of the groundwater velocity scaling factor generally lead to smaller ADEs. The greater variability in ADEs at 10^4 a compared with 10^5 a is due, as for tortuosity, to the fact that mobile contaminants are just beginning to discharge at the biosphere at 10^4 a for many simulations, whereas discharges are changing much less quickly at 10^5 a for most simulations.

Switch Selecting the Source of Domestic Water

This switch parameter selects the use of lake water or well water for the critical group. Its PDF is defined such that the well and the lake are each used in about 50% of the simulations (Davis et al. 1993). We can regard these two sets of simulations as simulations for two (assumed) mutually exclusive scenarios (Sections 2.1 and Chapter 4). Section E.6 in Appendix E discusses other switches, none of which strongly influences the maximum ADEs.

Figure 6-23 shows the effect of the switch selecting well water or lake water for domestic needs on the maximum ADEs up to 10^5 a. (Section E.6 of Appendix E shows similar plots for maximum ADEs from ^{129}I and ^{14}C.) The figure shows much weaker influences on the ADEs compared with the tortuosity of the lower rock zone and the groundwater velocity scaling factor. Comparison of the pairs of trend lines shows clearly that ADEs tend to be greater when the critical group uses the well instead of the lake.

The detailed analysis of the median-value simulation (Sections D.4 and D.8 in Appendix D) has shown that the well is important because it provides a source of water that is more contaminated than water from the lake. It potentially affects the critical group mostly through ingestion of contaminated drinking water and ingestion of contaminated food. Similar effects are expected to apply to most or all of the simulations in Figure 6-23. The presence or absence of the well is less important in sensitivity analysis of the probabilistic simulations than in the median-value simulation (Section D.8.2 in Appendix D) because the variation in ADEs resulting from changes in the other parameters obscures its effects.

6.5.5.4 Summary of the Probabilistic Sensitivity Analysis

The results described above and in Appendix E demonstrate that methods such as iterated fractional factorial analysis yield useful information even when dealing with a system model containing thousands of parameters, each of which may be characterized using a PDF. We are able to identify the important parameters and confirm that all have been found. We can also show statistically and graphically how an important parameter influences objective functions, such as the estimated annual doses. Finally, we can use results from the deterministic sensitivity analysis to explain why these influences occur.

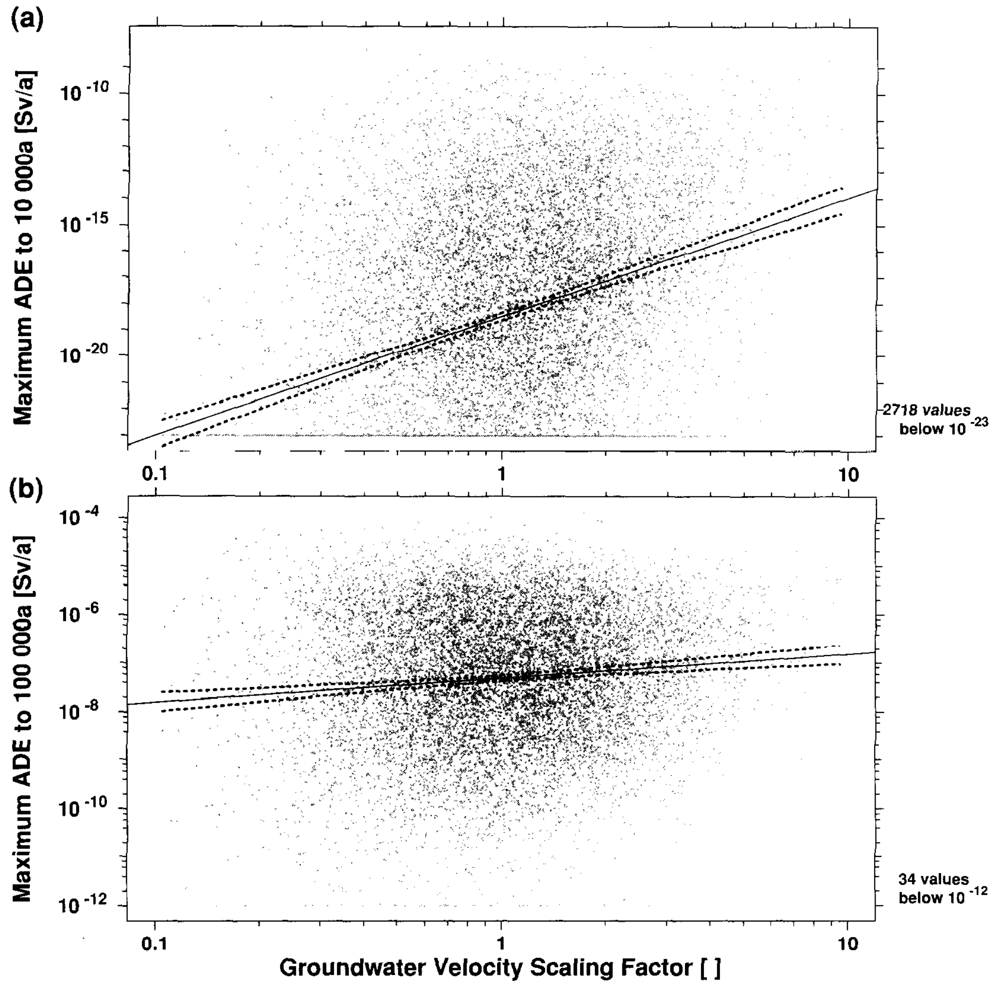

FIGURE 6-22: Effect of the Groundwater Velocity Scaling Factor on Maximum Annual Dose Estimates

The vertical axes show the maximum ADEs for times up to 10^4 a in part (a) and for times up to 10^5 a in part (b), and the horizontal axis shows the *groundwater velocity scaling factor* (a dimensionless parameter). Other comments are as for Figure 6-21. The correlation coefficients for the trend lines are 0.35 in (a) and 0.10 in (b).

These plots show that higher groundwater velocities generally result in larger estimates of maximum annual dose.

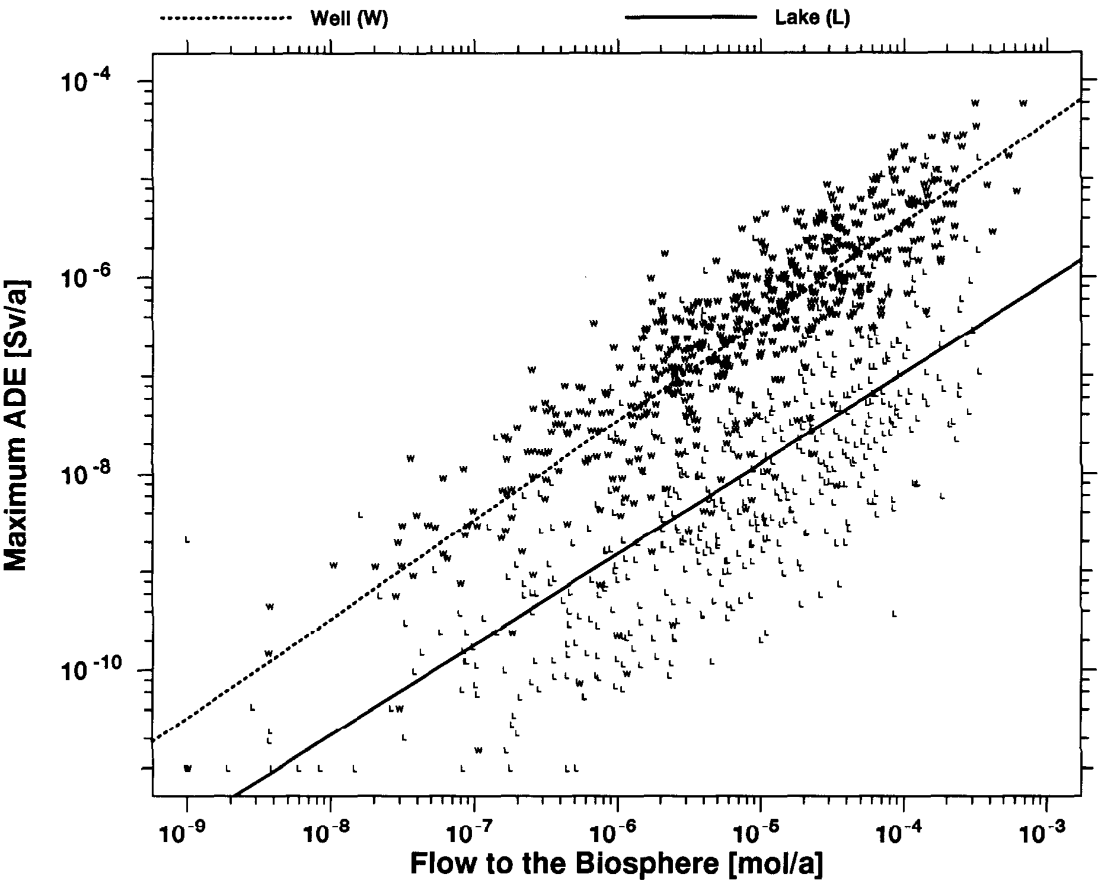

FIGURE 6-23: Effect of the Switch Selecting Source of Water on Maximum Annual Dose Estimates

The vertical axis is the maximum annual dose estimates for times up to 10^5 a. The horizontal axis is the estimated maximum (up to 10^5 a) flow of ^{129}I into the sediment and the well. (We plot all calculated data to display the range of estimates, even though some small values may not be meaningful.)

Results are shown for 1000 randomly sampled simulations. Each symbol plots the result of one simulation, with "L" and "W" identifying simulations involving the use of the Lake and the well. Two trend lines are shown: one for the lake and one for the well simulations. They are obtained by performing a least-squares fit to the logarithms of the data. The correlation coefficients for the trend lines are 0.85 for the simulations involving the well and 0.61 for the simulations involving the lake. The results show that dose estimates tend to be greater when the well is the source of domestic water.

For the reference disposal system modelled using SYVAC3-CC3, we have identified the parameters that most affect the maxima in the estimates of annual dose. Small differences occur when the results for the maxima for times up to 10^4 a and up to 10^5 a are compared. We can attribute these differences to a shift of importance from parameters that tend to delay impacts toward parameters that tend to attenuate impacts.

The two most important parameters discussed in this section are the tortuosity of the lower rock zone and the groundwater velocity scaling factor. The tortuosity is clearly the most important: its range of uncertainty has strong effects on both the magnitude and variability in the estimates of maximum dose (its importance tends to diminish from 10^4 to 10^5 a). The groundwater velocity scaling factor shows similar, although less pronounced effects. It is worthwhile to note that both of these parameters describe properties of the rock and water within the waste exclusion distance.

A third important parameter is the switch used to select from two (assumed) mutually exclusive scenarios, in which the source of water used by the critical group is either the well or the lake. The results for the reference disposal system show a clear trend: greater estimates of annual dose tend to occur when the source of water is the well. Thus, as noted in Sections 2.1 and Chapter 4, we can use switch parameters to combine several scenarios into a compound scenario in the postclosure assessment studies, and we can use sensitivity analysis to determine whether one of these scenarios leads to larger estimates of impact.

6.6 EFFECTS OF SELECTED SITE AND DESIGN FEATURES

6.6.1 Objectives and Method of Analysis

The studies described here are a special type of sensitivity analysis. They complement the analyses in Sections 6.3.3 and 6.5.5 and provide more information pertaining to the disposal concept. However, these studies are "special" because they use values for some parameters that are substantially different from those used in the assessment of the reference disposal system, and thus the results must be interpreted with caution.

These studies are focussed on two main issues:

- The identification of potential design constraints that could improve the performance of the disposal system. The studies of derived constraints described in Section 6.2 are based on variations of the median-value simulation. However, Section 6.5.1 shows that the effects of uncertainty are important and that the mean ADE is dominated by simulations with large ADEs. Thus we re-examine here the issue of derived constraints to test how the results in Section 6.2 would be affected when the effects of uncertainty are taken into consideration.

- The study of different assumed characteristics describing the reference site, to evaluate some features which might have a strong effect on estimated impacts.

The study of these selected site and design features involves special sets of 500 simulations. Each simulation corresponds to one of the first 500 randomly sampled simulations in the analysis of the reference disposal system, except for systematic changes to selected parameters that pertain to the site or design characteristic being examined. That is, for each study

- most parameters are assigned the same sequence of 500 randomly sampled values (identical to the first 500 randomly sampled values from the analysis of the reference disposal system); but

- a few parameters are assigned different values, chosen to display the effects of an assumed site or design feature.

This approach (called pairwise comparisons) includes the effects of parameter uncertainty, but at the same time we can observe small differences in effects that might be obscured using unique sets of randomly selected simulations or different methods of evaluation.

We focus the comparison on ADEs from three radionuclides: ^{14}C, ^{129}I and ^{99}Tc. Carbon-14 and ^{129}I were selected because they are major contributors to the total ADE. Technetium-99 was selected because it becomes an important contributor in some simulations described below. The ADEs are compared with the corresponding results from the first 500 randomly sampled simulations used in the analysis of the reference disposal system.

The following discussion summarizes the results of these comparisons. More details are provided in Section E.8 in Appendix E, including comments on the underlying reasons for the observed effects.

6.6.2 Summary of Cases Examined

Table 6-15 lists the thirteen cases studied, and the key assumptions made. Table 6-16 and Figures 6-24 and 6-25 summarize the results of the analysis. They show the arithmetic averages from 500 simulations of the maximum ADEs, where the maxima are taken over times up to 10^4 and up to 10^5 a. These averages are reported as ratios to the corresponding ADEs from the first 500 randomly sampled simulations used in the analysis of the reference disposal system.

Some results are radionuclide-dependent: Table 6-17 (and Figures E-39 to E-41 of Appendix E) show differences in the effects on the mean of the maximum ADEs from ^{14}C, ^{129}I and ^{99}Tc.

Ranked in (approximate) decreasing order of importance for their effects on the mean of the maximum ADEs to 10^5 a, the results in these tables and figures show that

- Eliminating vault rooms above fracture zone LD1 results in much smaller ADEs. Case 8 actually illustrates that adding vault rooms above LD1 leads to much larger mean ADEs (4 orders of magnitude at 10^4 a and 2 orders of magnitude at 10^5 a) relative to estimates for the reference disposal system. Although estimated doses attributed to ^{99}Tc are small, this radionuclide displays the largest relative effect.

TABLE 6-15

LIST OF THE ASSUMED SITE AND DESIGN FEATURES

Case	Assumption
1	Increased effective wall thickness (or corrosion allowance) of the titanium containers (from 4.2 to 8.4 mm)
2	More durable container (median container lifetime increased from about 4×10^3 a to about 6×10^4 a)
3	Increased thickness of the buffer (from 0.25 to 1.0 m)
4	Doubled effective thickness of the backfill (from 1.4 to 2.8 m)
5	Decreased groundwater velocities (by a factor of 2)
6	Greater concentrations of naturally occurring iodine in the groundwater (by a factor of 10)
7	Increased length of the waste exclusion distance (from about 50 to about 70 m)
8	Additional vault rooms included above fracture zone LD1
9	Nearby wells do not intersect the plume of contaminants
10	Compacted lake sediments are thicker (mean sediment thickness increased from 4.8 to 13.0 m)
11	Overburden is thicker (mean overburden thickness increased from 4.5 to 21.2 m)
12	Only organic soils are available for use by the critical group
13	Larger watershed for the lake (by a factor of 10)

Similar results are obtained from a comparison of cases with and without vault rooms above LD1 (Section E.8 of Appendix E), and for a waste exclusion distance of 70 m.

- Increasing the waste exclusion distance to about 70 m (Case 7) results in smaller mean ADEs, especially at 10^4 a where the reduction is 5 orders of magnitude. The effects at 10^5 a are more pronounced for ^{14}C and ^{99}Tc than for ^{129}I. (Section E.8 in Appendix E also shows that greater mean ADEs occur when the waste exclusion distance is decreased to about 30 m.)

- A more durable container (Case 2) is effective in reducing the mean ADEs, especially at 10^4 a where it is reduced to zero. The effects at 10^5 a are more pronounced for ^{14}C and ^{99}Tc than for ^{129}I.

- If the well does not contact the plume of contaminated groundwater (Case 9), the mean ADEs are reduced by a factor of 7 at 10^4 a and by a factor of 5 at 10^5 a. Technetium-99 is affected more than ^{14}C and ^{129}I.

TABLE 6-16

EFFECT OF ASSUMED SITE AND DESIGN FEATURES ON MEAN ADE*

Case Number and Description	Ratios** of the Means of the Maximum Estimated Annual Doses 10^4 a	10^5 a
1. Thicker container wall	0.24	0.93
2. More durable container	0.00	0.21
3. Thicker buffer	0.77	0.94
4. Thicker backfill	0.39	0.49
5. Decreased groundwater velocity	0.47	1.2
6. Greater concentrations of naturally occurring iodine in groundwater	0.17	0.23
7. Greater (70 m) waste exclusion distance	2.0×10^{-5}	0.14
8. Additional vault rooms above LD1	9.6×10^3	1.8×10^2
9. Well outside the contaminant plume	0.13	0.19
10. Thicker compacted lake sediment	0.94	0.86
11. Thicker overburden	0.89	0.77
12. Only organic soil in fields	1.9	1.5
13. Larger watershed	0.88	0.90

* The results in this table are based on similar sets of 500 randomly sampled simulations, except for differences in the values of the parameter(s) used to characterize the 13 cases listed in Table 6-15. For instance, in Case 1 (thicker container wall), the effective thickness of the reference titanium container is assumed to be 8.4 mm, or twice that used in the analysis of the reference disposal system (4.2 mm). In the 500 simulations for Case 1, all parameters are assigned values identical to those in the reference set, except that the effective thickness of the container is 8.4 mm.
The more durable container (Case 2) is most effective at 10^4 a, whereas a greater waste exclusion distance (Case 7) is most effective at 10^5 a.

** The values reported are ratios of arithmetic averages of the maximum (for times up to 10^4 a and up to 10^5 a) ADEs from the sets of 500 simulations: the mean from each of the 13 cases is divided by the corresponding mean from the first 500 simulations of the reference disposal system. A ratio less than unity for a case indicates it has a smaller mean maximum ADE compared with the corresponding mean maximum ADE from the reference disposal system.

- If there are larger levels of naturally occurring iodine in groundwater (Case 6), the mean ADEs that result from ^{129}I are decreased because of isotopic dilution (this process is discussed in Section 5.6.2.6, and its effects are described in Section E.6 in Appendix E). This case shows no effects, as expected, on the ADEs from ^{14}C or ^{99}Tc.

- Doubling the effective wall thickness of the container (Case 1) reduces the mean ADEs at 10^4 a by about a factor of 4. There is little effect at 10^5 a.

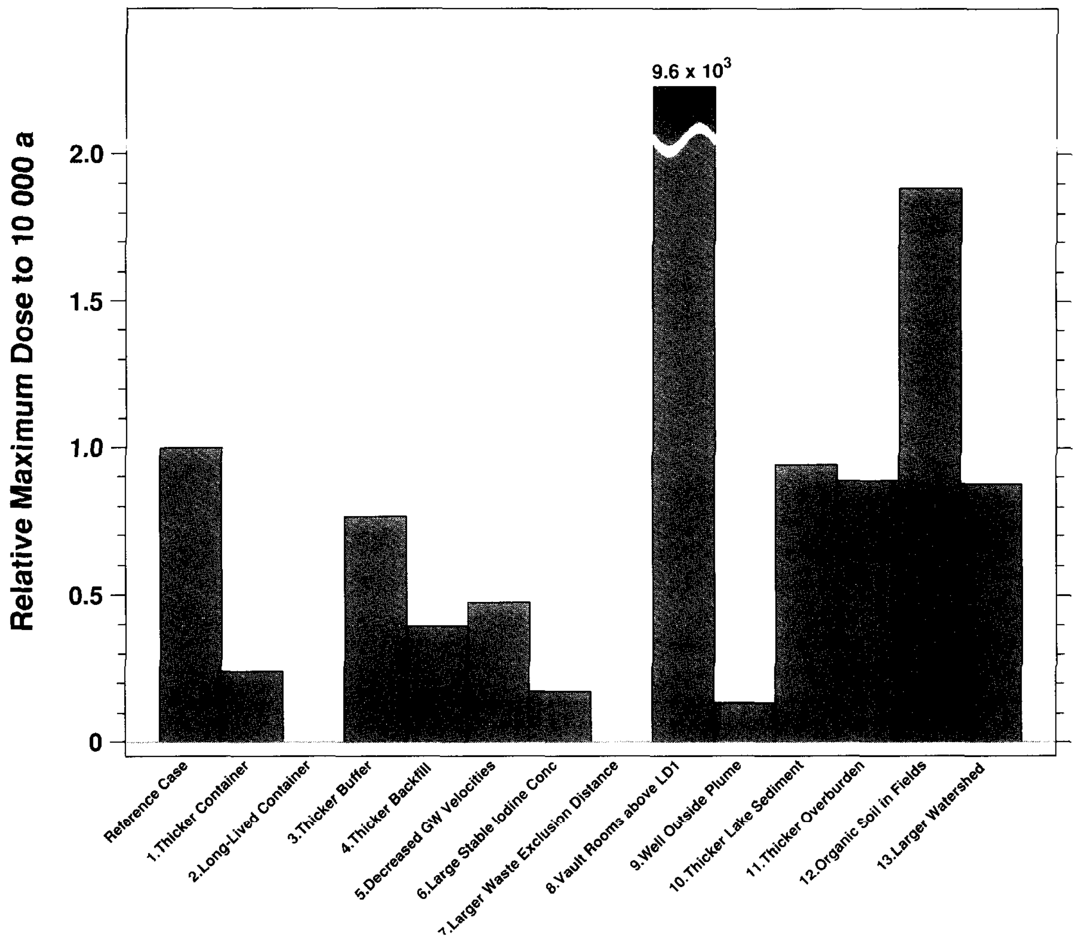

FIGURE 6-24: Effects of Assumed Site and Design Features on the Mean of the Annual Dose Estimates at 10^4 a

The results plotted are arithmetic averages of the maximum ADEs, for times up to 10^4 a, calculated from sets of 500 randomly selected simulations. The plots are shown relative to the reference case that is shown as the first bar on the left-hand side. The reference case corresponds to the arithmetic average of the maximum annual dose estimates to 10^4 a from the first 500 random simulations of the reference disposal system. The other bars show the effects of an assumed site or design feature. For example, Case 1 ("thicker container") refers to a study in which the thickness of titanium is twice its value in the reference disposal system, and Case 13 ("larger watershed") to a site whose watershed area is 10 times larger.
Cases 2 and 7 show the greatest decrease in the mean of the annual dose estimates; Case 8 shows the greatest increase (note that the top of the bar for Case 8 extends to 9.6×10^3, far beyond the scale of the vertical axis).

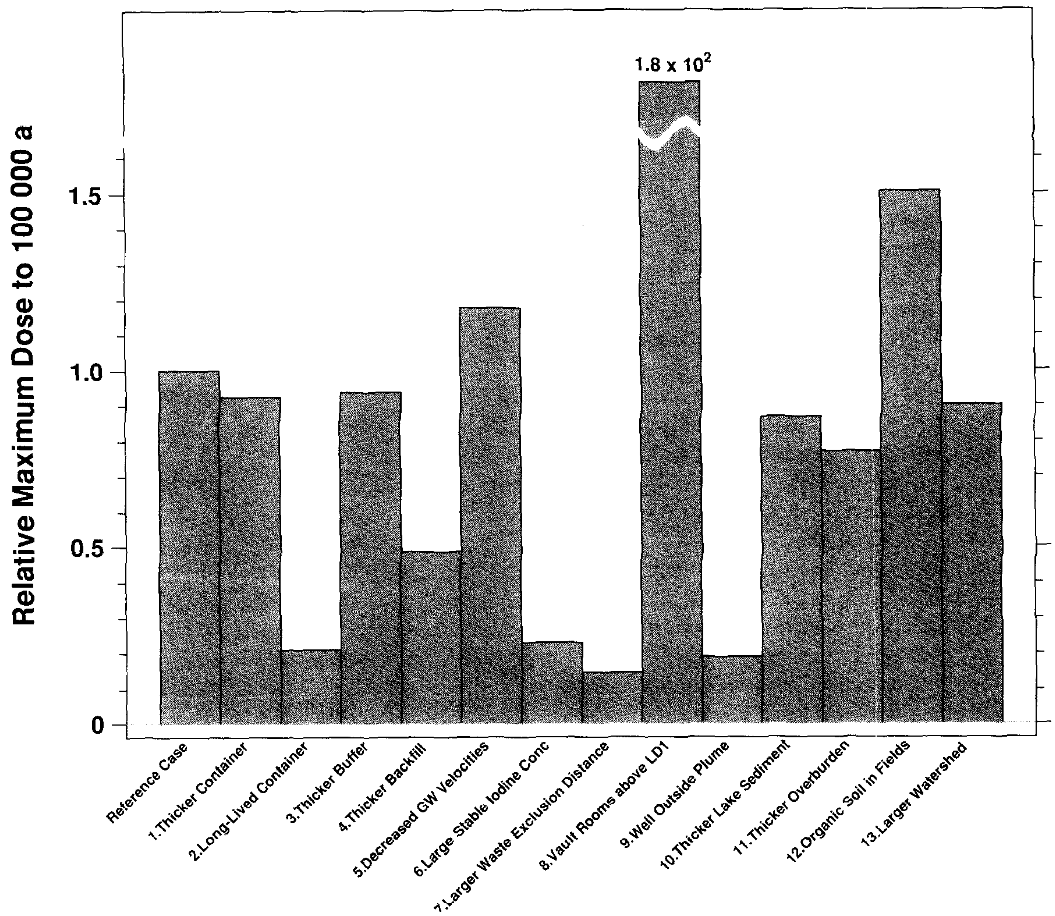

FIGURE 6-25: Effects of Assumed Site and Design Features on the Mean of the Annual Dose Estimates at 10^5 a

Comments are as for Figure 6-24, except that the data are for times up to 10^5 a. The first bar on the left-hand side is the reference estimate, and the other bars show the effects of an assumed site or design feature.
Cases 7 and 9 show the greatest decrease in the mean of the annual dose estimates; Case 8 shows the greatest increase (note that the top of the bar for Case 8 extends to 180, beyond the scale of the vertical axis). Data for this figure are taken from Table 6-16.

TABLE 6-17

EFFECT OF ASSUMED SITE AND DESIGN FEATURES ON ^{14}C, ^{129}I AND ^{99}Tc*

Case Number and Description	Ratio of Mean of the Maximum Annual Dose Estimates to 10^5 a from ^{14}C	^{129}I	^{99}Tc
1. Thicker container wall	0.65	0.93	0.52
2. More durable container	1.0×10^{-2}	0.21	2.2×10^{-3}
3. Thicker buffer	0.93	0.94	4.7×10^{-8}
4. Thicker backfill	0.45	0.49	3.7×10^{-6}
5. Decreased groundwater velocity	0.53	1.2	0.12
6. Greater concentrations of naturally occurring iodine in groundwater	1.00	0.23	1.00
7. Greater (70 m) waste exclusion distance	3.2×10^{-2}	0.14	1.8×10^{-3}
8. Additional vault rooms above LD1	4.8×10^{2}	2.2×10^{1}	9.1×10^{12}
9. Well outside the contaminant plume	0.18	0.19	1.6×10^{-2}
10. Thicker lake compacted lake sediment	0.96	0.87	0.99
11. Thicker overburden	0.83	0.77	0.99
12. Only organic soil in fields	10.	1.5	15.
13. Larger watershed	0.86	0.90	1.00

* Comments are as for Table 6-16, except that the data are for ^{129}I, ^{14}C or ^{99}Tc. The values reported are ratios of arithmetic means of the maximum annual dose estimates, up to 10^5 a, resulting from ^{14}C, ^{129}I or ^{99}Tc. The ratio is the mean estimated from the 13 cases divided by the mean estimated from the reference set. A ratio less than unity means the corresponding case has a smaller annual ADE.

Case 8 is the most sensitive feature: adding vault rooms above LD1 leads to large increases in estimated dose. The results indicate that some assumed site and design features have different effects on different radionuclides. For ^{14}C, the more durable container (Case 2) is most effective; for ^{129}I it is a greater waste exclusion distance (Case 7); and for ^{99}Tc it is a thicker buffer (Case 3).

- Doubling the amount of backfill present (Case 4) reduces the mean ADEs by about a factor of 2. There is a strong attenuation in the ADEs due to ^{99}Tc.

- If groundwater velocities are everywhere smaller by a factor of 2 (Case 5) there is a mixed effect: the mean ADEs are reduced by a factor of 2 at 10^4 a but increased slightly at 10^5 a. Results in Table 6-17 show that the maximum of the ADEs up to 10^5 a are increased for ^{129}I and decreased for ^{14}C and ^{99}Tc.

- Increasing the buffer thickness (Case 3) slightly reduces the mean ADEs at 10^4 and 10^5 a, although there is an extremely strong attenuation in the ADEs due to ^{99}Tc (approximately 7 orders of magnitude at 10^5 a).

- If the local water bodies have a larger watershed (Case 13) the mean ADEs are only slightly smaller. Thicker compacted lake sediment and thicker overburden have little effect (Cases 10 and 11).

- If only organic soils are available (Case 12) the mean ADEs increase by less than a factor of 2, with the largest effects on ^{14}C and ^{99}Tc.

6.6.3 Conclusions

Of the 13 assumed site and design features, the most effective in reducing the mean ADEs for times up to 10^5 a involve

- eliminating the vault rooms above fracture zone LD1, where the groundwater velocities are higher and directed downwards and away from the backfill; and

- maximizing the waste exclusion distance.

These observations are derived from a probabilistic analysis that takes into account the effects of uncertainty. Both these constraints were also identified in Section 6.2 from the analysis of the median-value simulation and were used to finalize the design of the reference disposal system.

Note that these two design constraints are for the reference disposal system that is characterized using site-specific information from the WRA and that assumes a particular design, layout and depth for the hypothetical disposal vault. Nonetheless, equivalent design constraints could also be important for an actual disposal facility at another site.

The analyses discussed above have considered each case separately, but it would be feasible to employ two or more and achieve even better performance. For example, the results in Table 6-17 imply that impacts attributed to ^{129}I would be substantially reduced when using a more durable container and a greater waste exclusion distance.

Moreover, when considering more durable containers, the design of the entire reference disposal vault need not be modified. On the basis of the results described previously and in Appendices D and E, the principal exposure pathways originate from the vault sectors nearest fracture zone LD1. Thus results similar to those in Table 6-16 and 6-17 would be obtained if, for example, the use of more durable containers were limited only to vault sectors 10 to 12.

6.7 ANALYSIS OF THE OPEN-BOREHOLE SCENARIOS

6.7.1 Overview

The probability of occurrence and potential consequences of an open borehole would be strongly dependent on site-specific properties. Thus we have focussed our analysis on the reference disposal system.

In addition, the probability that an open borehole remains open at the time of closure would depend on the quality assurance measures followed by the implementing organization during all stages of the disposal project. For the reference disposal system, we believe the application of three quality assurance procedures would result in an extremely small probability of occurrence. In fact, we conclude the probability is so small that the open-borehole scenarios would not contribute significantly to the radiological risk associated with the reference disposal system.

In the following discussion, we first describe the open-borehole scenarios and discuss their likelihood of occurrence. We then examine potential impacts, based on an analyses of results from SYVAC3-CC3.

6.7.2 Description of the Open-Borehole Scenarios

These scenarios describe a situation in which one or more open boreholes penetrate the geosphere barrier and provide a potentially significant transport pathway for contaminants in the disposal vault. Project records would give the location, orientation and depth of all boreholes, and project procedures would ensure a borehole is sealed once it is no longer required. However, the possibility must be examined that a borehole remains open at the end of the project. For example, the location of a borehole may not be known because of lost or damaged records, because of inaccurate surveying procedures, or because of calculation or data transcription errors.

Figure 6-26 illustrates the unique factor defining these scenarios: an open borehole passes through the rock near a vault room containing nuclear fuel waste. We evaluate the situation where:

- the borehole extends downwards from the surface through fracture zone LD1 and reaches the depth of the disposal vault;

- the location of the borehole at the surface is not known, and thus it is not used as a water-supply well, although it may affect and be affected by nearby water-supply wells (especially wells that intercept fracture zone LD1);

- the borehole was drilled prior to closure of the disposal vault; and

- the borehole is open at the time of vault closure.

In addition, the open-borehole scenarios include all the factors represented in the SYVAC3-CC3 system model. For example, the disposal vault contains 162 000 Mg U, about 50 m of sparsely fractured rock separates any

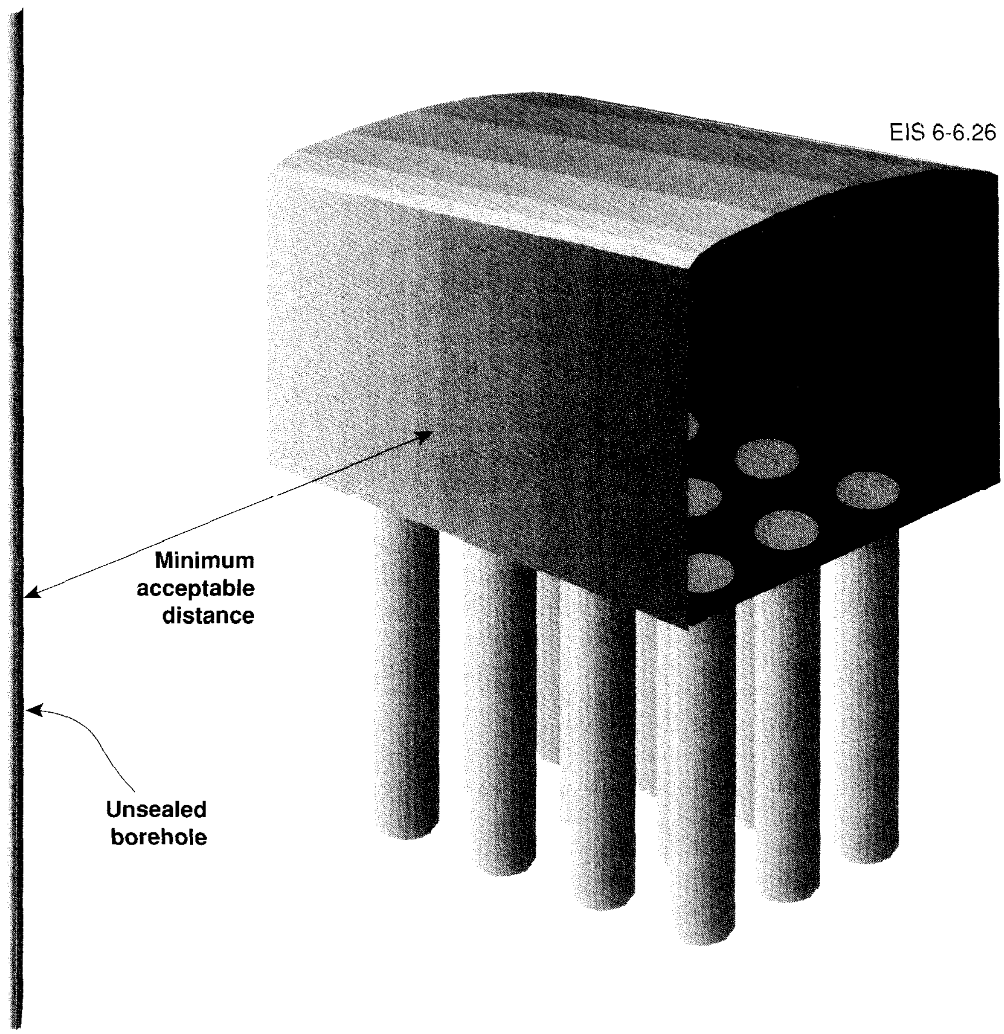

FIGURE 6-26: Feature of Interest for the Open-Borehole Scenarios

These scenarios deal with an open borehole that passes near the vault and extends upwards to the surface. Our analysis indicates that the open-borehole scenarios would have an extremely small probability of occurrence for the reference disposal system because of the application of three quality assurance procedures. These procedures would be in force during the project, and would be aimed at minimizing the likelihood that a borehole would remain open at the time of vault closure. They involve ensuring all boreholes are properly sealed, isolating vault rooms containing nuclear fuel waste from any deep boreholes by some minimum acceptable distance, and confirming there are no open boreholes near any vault room. We believe that these procedures would be sufficiently effective such that the open-borehole scenarios would not contribute significantly to the radiological risk.

vault room containing waste and fracture zone LD1, a water-supply well intercepts LD1 along the centre of the pathways of any contaminants moving up fracture zone LD1, and the critical group obtains all its food and water from local sources. (Moreover, we consider just one open borehole. However, its probability of occurrence is so small that the probability of occurrence of two such boreholes would be insignificant.)

Finally, for the reference disposal system, we make the following assumptions that exclude certain types of boreholes.

- We assume that no boreholes were drilled prior to the start of the project. Any such boreholes would have been drilled to search for minerals or to construct water-supply wells. However, the rock in the vicinity of the reference disposal system (that is, the rock near the Underground Research Laboratory in the WRA) is of little interest for mineral exploration, and there are abundant nearby sources of surface and near-surface water. In addition, water-well drilling records and local residents indicate no deep boreholes have been previously drilled in the area.

- We assume that no unsealed boreholes were drilled into the surrounding rock from a vault room containing emplaced nuclear waste. During the construction stage, many boreholes may be drilled underground, but we presume that construction procedures will preclude the drilling of any boreholes from within a vault room, other than those boreholes used to construct the vault room (and which would be confined to the excavated rock mass). We also presume that boreholes drilled for site characterization purposes would either start at the surface or from vault tunnels that are remote from any vault room used for disposal. Our following analysis deals with boreholes starting from the surface, but similar comments and conclusions would apply to boreholes that start from underground tunnels.

- We assume that no boreholes were drilled after closure of the vault. We evaluate the impacts of these boreholes in the inadvertent human intrusion scenarios (Section 6.8).

6.7.3 Probability of Occurrence of the Open-Borehole Scenarios

Exploration boreholes would be drilled during all stages of the project, beginning during site characterization and continuing through to extended monitoring. However, only a few such boreholes would extend from the surface to the depth of the reference disposal vault. The number of boreholes deeper than about 500 m would depend on the characteristics of the site. Typically, about 20 such boreholes would be drilled from the surface in the area of a disposal vault.

Three quality assurance procedures would be implemented during the project to minimize the possibility that a borehole would remain open at the time of vault closure.

1. *Ensure that all boreholes are properly sealed.* This procedure would be in effect during all stages of the disposal project, starting with the first

borehole drilled during the siting stage and concluding when the last borehole has been sealed in the closure stage. The procedure would involve engineering surveys to locate precisely all boreholes; a dedicated records management system to ensure that information on the location, orientation, depth, purpose and usage is always available; and a requirement to seal a borehole once it is no longer required. Cross checks between borehole drilling records and borehole sealing records would be used to confirm that all boreholes have been sealed at the time of closure of the disposal vault. Special attention would be given to the deep boreholes that pass near the disposal vault.

2. *Avoid locating any vault room containing nuclear waste within some minimum acceptable distance of all deep boreholes.* This procedure would be in effect during the construction stage of the project. The minimum acceptable distance would be defined such that the impacts would be insignificant even if there were an open borehole in the most unfavorable location and at that minimum distance.

   Our analysis, described in Section 6.7.4, indicates there would be no significant contribution to risk for the reference disposal system if an open borehole were about 30 m distant from any room containing waste. That is, a minimum acceptable distance for the reference disposal system is about 30 m. In fact, the 30-m distance is based on available results from SYVAC3-CC3, and not on a dedicated analysis; it is likely that a smaller distance would provide sufficient isolation.

3. *Confirm that there are no open boreholes near any vault rooms containing nuclear fuel waste.* This procedure would be in effect during the operation stage of the disposal project. It would be achieved using geophysical scanning surveys, such as ground penetrating radar or seismic reflection, to detect the presence of nearby open boreholes. Present day survey methods can detect unsealed boreholes passing within 5 m of underground excavations in rock saturated with saline groundwater (Holloway and Mugford 1990; Holloway et al. 1986; Olsson et al. 1987), and the detection distance is greater if the groundwater is less saline. We expect that these geophysical survey technologies will continue to improve.

A borehole could remain open at the time of vault closure and affect the integrity of the reference disposal system only if there was a failure in all three quality assurance procedures: a failure to seal the borehole, a failure to isolate the disposal vault from all deep boreholes by about 30 m, and a failure to detect the presence of the borehole near a vault room containing waste. We believe that this possibility is unlikely: the three redundant quality assurance procedures would provide a high degree of confidence that no boreholes would remain open at the time of vault closure that could have a significant effect on the performance or safety of the reference disposal system. Thus we conclude that the open-borehole scenarios would not make a significant contribution to the radiological risk for the reference disposal system.

6.7.4 Potential Impacts of the Open-Borehole Scenarios

In this section, we provide support for the "minimum acceptable distance" of 30 m mentioned in Section 6.7.3. In addition, we examine potential impacts associated with an open borehole.

Chan and Stanchell (1992) used a detailed hydrogeological model of the hypothetical reference disposal system to simulate the effect of an unsealed borehole on the groundwater flow fields. Their analysis assumed that the rock between the borehole and the disposal vault is homogeneous and sparsely fractured, with properties of the bulk rock at 500 m depth. They concluded that effects on the groundwater flow fields in the rock surrounding the disposal vault would be relatively localized, extending at most a few tens of metres away from the borehole. These effects would also be dependent on the possible presence of a nearby water-supply well, and the rate of groundwater withdrawal from the well. Their results also indicated that the transport of contaminants from the vault could be significantly increased if the unsealed borehole was situated very close to a room containing nuclear fuel waste (Chan and Stanchell 1992).

From these results, we expect the impacts associated with the open-borehole scenarios would be similar to those estimated using the SYVAC3-CC3 system model but with some *additional* impacts that would be attributed to the localized effects of the open borehole.

We analyze results from SYVAC3-CC3 to estimate an upper bound on the additional radiation dose to a member of the critical group. The discussion in Section 6.5.2 shows that the estimated mean annual dose for the SYVAC scenarios reaches a maximum value of 1.0×10^{-11} Sv/a for times up to 10^4 a. Moreover, our sensitivity analysis attributes this radiation dose to the transport of radionuclides from vault sectors 10, 11 and 12 to the permeable fracture zone LD1 about 50 m away. That is, the engineered barriers and 50 m of low-permeability sparsely fractured rock between the vault and LD1 lead to very small estimates of annual dose. These estimates provide an upper bound on the additional impacts that might be associated with an open borehole located 50 m away from a vault room containing waste.

In fact, we expect that an open borehole located 50 m from the vault would have much smaller impacts than an extensive fracture zone located 50 m from the vault, because the effects of an open borehole would be much more localized and because the fracture zone provides a much greater flow of groundwater and contaminants from the vault to the biosphere than an open borehole. Thus the additional annual dose associated with an open borehole that is 50 m from a vault room containing waste is certainly less than 1.0×10^{-11} Sv/a for times up to 10^4 a.

More information is available from other results produced by SYVAC3-CC3. For example, the studies of derived constraints in Section E.8 of Appendix E, which use 500 randomly sampled simulations, indicate that the additional annual dose associated with an open borehole that is 30 m from a vault room containing waste would be less than approximately 10^{-9} Sv/a for times up to 10^4 a.

These results from SYVAC3-CC3 indicate that radiation doses associated with open boreholes would meet the dose associated with the AECB risk criterion, provided that no borehole were within some minimum acceptable distance from any vault room containing nuclear waste. For the reference disposal system, the minimum acceptable distance is certainly no more than 30 m, and it likely would be much smaller.

We have also examined one special simulation using SYVAC3-CC3 to obtain an estimate of the effects of an open borehole. In this simulation, we modified the network of segments in the geosphere model so as to approximate the presence of an open borehole that is separated from the vault rooms by only 5 m of sparsely fractured rock (Davison et al. 1994b). We assume this borehole is potentially exposed to the entire inventory of nuclear waste found in two adjacent vault rooms. The borehole extends upwards to the surface and passes through fracture zone LD1. We have chosen a conservative orientation for the borehole: it reaches LD1 at a point approximately 800 m upstream of the intersection of the LD1 and a water-supply well used by the critical group, and it is aligned to lie in the centre of the plume of contaminated water that would be released from the disposal vault and that would be captured by the well. With this modified network of segments, the withdrawal of water from the well enhances the movement of groundwater and contaminants from the disposal vault to and up the open borehole. Moreover, all contaminants that enter the open borehole would be eventually captured by the well. For this study, all parameters were fixed at their median values and we estimated the annual dose that would arise from ^{14}C, ^{135}Cs, ^{129}I, ^{59}Ni, ^{107}Pd, ^{79}Se and ^{99}Tc from used fuel. Results show that the estimated annual dose rises to a value of 4×10^{-6} Sv/a at 10^4 a, or about 10% of the annual dose associated with the AECB risk criterion.

The results of this special simulation suggest that an open borehole would not produce a large annual dose, even if it passed as close as about 5 m from the reference disposal vault.

6.8 ANALYSIS OF THE INADVERTENT HUMAN INTRUSION SCENARIOS

6.8.1 Overview of the Analysis for the Intrusion Scenarios

In the scenario analysis for the reference disposal system (Chapter 4), we identified only one disruptive event that could significantly affect the integrity of the reference disposal system over 10^4 a. It is inadvertent human intrusion into the disposal vault caused by activities such as exploration drilling and mining.

The probability of occurrence of an intrusion event is expected to be small. Merrett and Gillespie (1983) concluded that activities leading to inadvertent human intrusion into a disposal vault would be unlikely because the vault is relatively small compared with the total area of the Shield, it is located at a great depth, and it would be sited in rock that is of low economic value. This last consideration constitutes an important siting consideration for a disposal vault (Davison et al. 1994a).

Wuschke (1991, 1992) estimates the probability is less than 5×10^{-6} that an intrusion event (of the type described below) would lead to significant radiation exposure, for all times up to 10^4 a. The joint probability of occurrence of two or more independent events is given by the product of their individual probabilities and is even smaller. Thus the probability of occurrence of two such intrusion events would be less than 25×10^{-12} for all times up to 10^4 a. We assume, therefore, that there is no need to consider the occurrence of two or more such events.

We have determined that a practical approach to evaluating a low-probability scenario is to treat it separately from high-probability scenarios. Thus we have not included the factor for inadvertent human intrusion in the SYVAC scenarios, and we do not estimate impacts for human intrusion using the system model in SYVAC3-CC3. (If we were to include in SYVAC3-CC3 an event whose probability of occurrence is 10^{-6}, we would need to perform more than 3 million randomly sampled simulations to be confident (at the 95% level) that the event would have been selected in at least one simulation (Andres 1986).) Instead we use results from Wuschke (1991, 1992), who evaluated impacts for inadvertent human intrusion using the system model outlined in Section 6.8.4 and based on the GENII code (Napier et al. 1988).

We believe the models and data used in the analysis yield overestimates of the risks for the inadvertent human intrusion scenarios. We then use these calculated risks for comparison with the AECB risk criterion. It may be misleading, however, to compare the risks estimated for the inadvertent human intrusion and SYVAC scenarios because their analyses are based on different system models.

6.8.2 Description of the Inadvertent Human Intrusion Scenarios

The human intrusion scenarios are defined as radiation exposures initiated by human actions at the disposal site, following closure of the facility. These actions could be deliberate or inadvertent. We are concerned here with actions that are unintentional, or inadvertent, in the sense that they are carried out without knowledge of the presence of a disposal vault and its potential hazards.

Wuschke (1991, 1992) has classified inadvertent human intrusion into five categories:

- exposure to undispersed waste,
- exposure to waste dispersed by previous intrusions,
- human-induced alteration of the expected evolution of the disposal system,
- contact with a contaminated groundwater plume, and
- contact with materials contaminated by the groundwater plume.

The last three categories are evaluated in the SYVAC scenarios. For example, the analysis described in Sections 6.2 to 6.6 includes consideration of bedrock wells used to supply the critical group with domestic water and with irrigation water, and these wells intercept the contaminated groundwater plume moving up fracture zone LD1. Thus members of the critical group may contact a contaminated groundwater plume used as a source of domestic water. They may also contact materials contaminated by the plume, such as food from their garden, which is irrigated with well water, and produce from animals that drink contaminated well water. Moreover, analysis of the SYVAC scenarios includes cases where these wells may withdraw more than 10^4 cubic metres of water per year. These large rates of water withdrawal would significantly perturb existing groundwater flow patterns around and above the hypothetical disposal vault (Reid and Chan 1988, Reid et al. 1989, Davison et al. 1994b).

The discussion here is focussed on inadvertent human intrusion associated with the first two categories, involving exposure to dispersed and undispersed waste. We make extensive use of the analysis by Wuschke (1991, 1992), who evaluated four inadvertent human intrusion scenarios that are:

> ...considered likely to present the highest risk to the intruder, i.e., those likely to have the highest product of probability and consequence. Each scenario selected is generally representative of a set of similar scenarios with lower probability or consequence. All of the scenarios analyzed would be initiated by a drilling operation that penetrates the waste and brings it to the surface. (Wuschke 1991).

Each of these four closely related intrusion scenarios starts from the same initiating event, and the main differences pertain to the characteristics of the humans most at risk.

Wuschke (1991,1992) analyzed two scenarios involving exposure to undispersed waste:

- The first, called the drill-crew exposure scenario, deals with the slurry of pulverized rock, nuclear fuel waste and other material brought to the surface with the drilling fluid. It examines the radiation dose that would be received by a member of the drilling crew, exposed both to external radiation and to inhalation of dust from the slurry.

- The second, called the core-examination scenario, deals with relatively large pieces of rock, nuclear waste and other material removed as a drill core. It examines the radiation dose that would be received by a laboratory technician, exposed to external radiation and inhalation and ingestion of dust arising from preparation and examination of the drill core.

Two other cases were also analyzed in which it is assumed the extracted waste from a drilling operation is dispersed and left on the drilling site (Wuschke 1991, 1992):

- The construction scenario deals with a construction worker who contacts the waste when working at the site and who is exposed both to external radiation and to inhalation of contaminated dust.

- The resident scenario deals with a person who lives in a house built on the drilling waste and who is exposed through external radiation, inhalation of contaminated dust, and ingestion of food obtained from contaminated soil.

6.8.3 Probabilities of Inadvertent Human Intrusion

The following discussion indicates that the probabilities of these scenarios are relatively small, in part because of the characteristics of deep geological disposal of nuclear fuel waste: deep burial reduces the possibility of human intrusion by isolating the waste far from human communities in a massive geological barrier. Our analysis assumes, however, that a sequence of events may occur that by-passes all of these natural and engineered barriers.

Wuschke (1991, 1992) used an event-tree methodology as a framework for defining probabilities of occurrence for the drill-crew, core-evaluation, construction and resident scenarios. Each scenario implies that a series of events occurs, such as selecting a drilling site, missing controls or warnings about the vault, and continuing drilling to vault depth. The event tree considers the sequence of events that would lead to each of the intrusion scenarios; the events and associated probabilities were based on the judgments of experts in relevant technologies and social sciences (Wuschke 1992). For example, the drill-crew and core-examination scenarios include the following events (Wuschke 1992).

- A proposal is made to drill a borehole on the disposal site to the depth of the vault. The assumed probability of occurrence of this event is 4×10^{-4} boreholes per year, based on a vault area of 4×10^{6} m^2 and using a value of 10^{-10} boreholes$\cdot m^{-2} \cdot a^{-1}$ for the areal frequency of a proposal to drill to a depth greater than 500 m in the vicinity of the disposal vault.

- Active institutional controls, such as security and surveillance measures continuing after closure of the facility, do not stop the drilling. The assumed probability is time-dependent: it is zero at the time of closure of the vault and slowly increases to unity after 500 a, reflecting a presumed gradual decline in the effectiveness of active controls.

- Passive institutional controls, such as long-lasting site markers, records and archives, do not stop the drilling. The assumed probability is also time-dependent, slowly increasing from zero at the time of closure of the vault to a value of unity after 2×10^{3} a, and presuming a gradual decline in the effectiveness of passive controls.

- Drilling is not prevented by detection of the disposal vault during pre-drilling investigations. The assumed probability is 0.5.

- The borehole intersects a container. The assumed probability, 1.1×10^{-2}, is based on the ratio of areas of the containers and the disposal vault.

The probability of occurrence of an intrusion scenario is given by the product of the probabilities of its constituent events. Wuschke (1992) estimates that the probabilities of occurrence of the four intrusion scenarios are zero at the time of closure of the vault and slowly increase thereafter, with maximum probabilities of less than 5×10^{-6} for all times up to 10^4 a. In addition, results from Wuschke (1992) indicate that

- The probabilities of occurrence of the drill-crew and core-examination scenarios reach their maximum values at (approximately) 2×10^3 a, because the probabilities of their constituent events have reached their time-independent upper limits.

- The probabilities of occurrence of the construction and resident scenarios continue to increase at a slow rate for times up to and past 10^4 a, because these probabilities take into consideration the cumulative probability that waste may have been extracted by drilling in prior years and left at the site.

6.8.4 Consequences of Inadvertent Human Intrusion

Wuschke (1992) estimated the radiation doses for the four inadvertent human intrusion scenarios using the pathways-analysis computer code GENII (Napier et al. 1988). The analysis considered inhalation, ingestion and external exposure pathways and used parameter values recommended by the ICRP (1979) for the calculation of dose. The analysis also required other biosphere pathways parameters, such as occupancy time and area of dispersion of extracted waste; values for these parameters were based on the judgment of specialists in related disciplines (Wuschke 1992).

For all four scenarios, the estimated radiation doses were largest at earlier times, when the waste is most radioactive. Some estimated annual doses exceeded 1 Sv/a for the resident and drill-crew exposure scenarios. Wuschke (1991) notes "this is not surprising, since nuclear waste is isolated in a disposal facility because of its potential to cause such doses." The important pathways and radionuclides vary both with time and with the scenarios (Wuschke 1992):

- For the drill-crew exposure scenario, estimated doses are initially dominated by external exposure to ^{137}Cs and ^{60}Co. Inhalation pathways are more important after about 3×10^2 a, and the largest contributors include ^{241}Am, ^{129}I, ^{239}Pu and ^{14}C.

- For the core-examination scenario, inhalation of ^{241}Am dominates exposures up to about 10^3 a, followed by ingestion of ^{240}Pu and ^{239}Pu at longer times.

- For the construction scenario, external exposure to ^{137}Cs is most important for the first 50 a, followed by inhalation of ^{241}Am and ^{239}Pu at longer times.

- For the resident scenario, ingestion of ^{90}Sr and ^{241}Am are most important up to about 200 a, Ingestion pathways are also most important for times beyond about 4×10^3 a, with contributors such as ^{129}I. Inhalation dominates the intermediate times, and the main contributors to dose are ^{241}Am, ^{240}Pu and ^{239}Pu.

The largest estimated doses were obtained for the resident scenario for the first 3 x 10^2 a, followed by the core-examination scenario for longer times (Wuschke 1992).

6.8.5 Risk of Inadvertent Human Intrusion

The radiological risk associated with the inadvertent human intrusion scenarios is calculated using the equation prescribed by the AECB (1987a). In this equation, the radiological risk attributed to an individual scenario is the product of its probability of occurrence, its associated dose consequence, and the risk conversion factor. As noted in Section C.4 in Appendix C, we use a modified calculation when estimated annual doses exceed 1 Sv/a and assume the risk is (numerically) equal to the probability of occurrence of the scenario.

Figure 6-27 shows our calculated risk-time curves for the four intrusion scenarios. Most of the calculations of risk are made directly from the estimates of probabilities and annual doses documented by Wuschke (1992). However, interpolation of Wuschke's results were required for the drill-crew and resident scenarios because their estimated annual doses decrease downwards through 1 Sv/a at early times. The interpolations were used to estimate the time at which annual doses reached 1 Sv/a and to estimate the corresponding probabilities. These interpolated data produce the two discontinuities in the risk-time curves, one near 40 a for the drill-crew exposure scenario, and the other near 150 a for the resident scenario. (These discontinuities are related to the modified calculation for risk, discussed in Section C.3 of Appendix C. The corresponding risk curves reported by Wuschke (1991, 1992) are based on the risk equation from the AECB (1987a) and are different only at the earlier times where estimated annual doses exceed 1 Sv/a.)

Figure 6-27 shows that the largest calculated risks are associated with the drill-crew and resident scenarios and both reach peak values of about 3 x 10^{-10} serious health effects per year. Smaller risks are associated with the core-examination and construction scenarios.

The radiological risk for each scenario applies to an individual who may belong to a different critical group. That is, it is likely that no one individual would be a member of the drilling crew, a laboratory technician, a construction worker and a resident, all at the same time. However, it is conservative to assume that the same individual does belong to all four critical groups and sum the risks from the four scenarios to obtain a total risk. The maximum of this total is about 3 x 10^{-10} serious health effects per year.

The calculated risks for each scenario decrease at longer times because of the competing trends of probability of occurrence and estimated dose. After 2 x 10^3 a, when active and passive institutional controls are assumed to be ineffective, the estimated probability of occurrence of each scenario is at its constant maximum value (for the drill-crew exposure and core-examination scenarios) or is increasing at a small rate (for the construction and

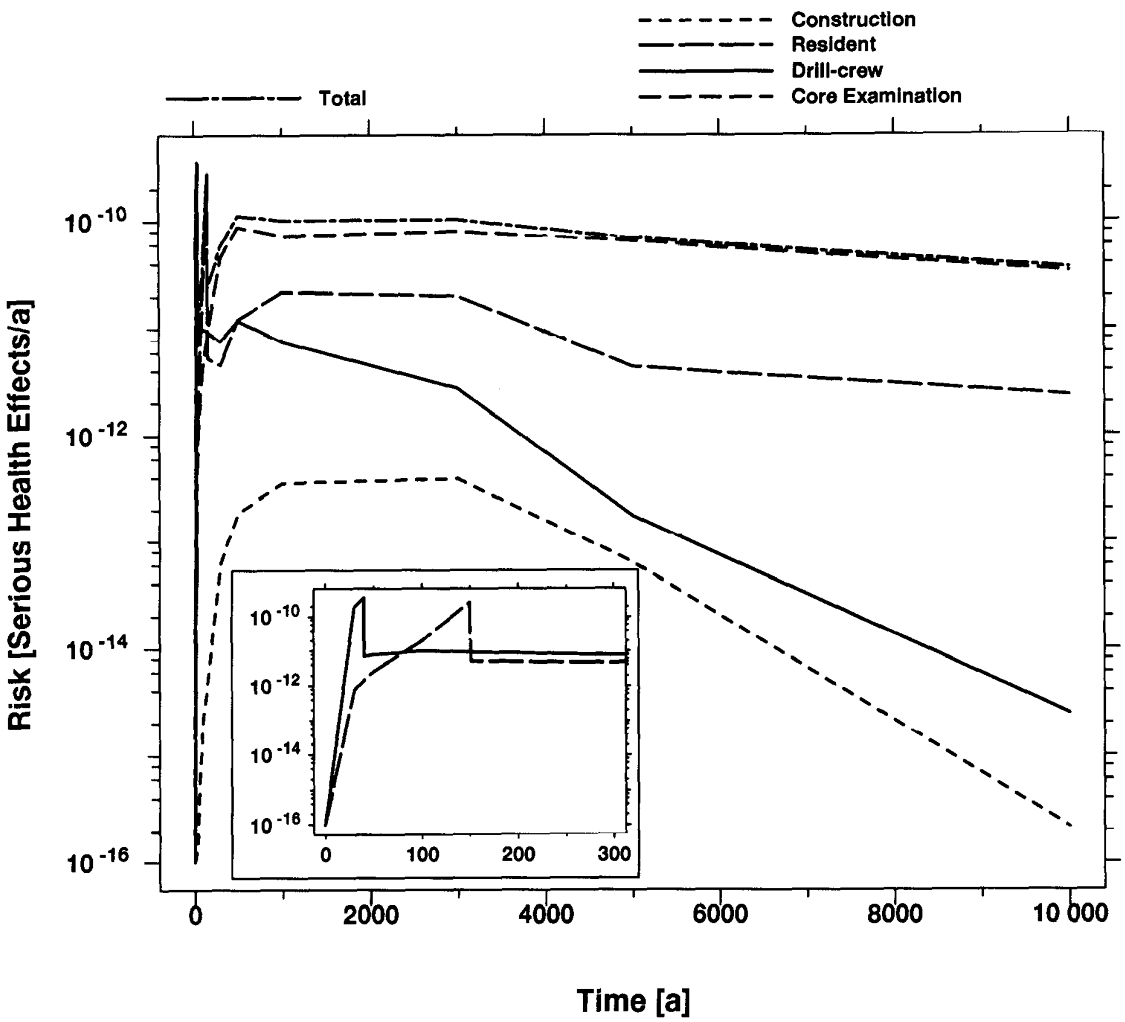

FIGURE 6-27: Risk from Inadvertent Human Intrusion Scenarios

The four lower curves show the calculated radiological risk for the drill-crew exposure, core examination, construction and resident scenarios, and the upper "total" curve is their sum. The maximum in the radiological risk for each curve (and the sum of the risk for the four curves) is at least 3000 times smaller than the AECB risk criterion of 10^{-6} fatal cancers and serious genetic effects in a year (AECB 1987a).

The inset shows a blowup, for times up to 300 a, of the curves for the drill-crew and resident scenarios. The calculation of risk uses a modification of the AECB equation (1987a) which leads to discontinuities in the risk-time curve if estimated annual doses pass through 1 Sv/a. Two such discontinuities are more obvious in the blowup: one near 40 a for the drill-crew scenario and and one near 150 a for the resident scenario.

resident scenarios). However, the estimated doses for each scenario are decreasing faster than their probabilities are increasing. Consequently, after about 5 x 10^2 to 3 x 10^3 a, the calculated risks for each scenario are decreasing, and continue to decrease for times up to 10^4 a. The radiological risks calculated for each of these scenarios (and their sum) are more than 3000 times smaller than the AECB risk criterion of 10^{-6} serious health effects per year (AECB 1987a), at any time over the first 10^4 a following closure of the disposal vault.

We conclude that, although human intrusion can by-pass all natural and engineered barriers, the calculated radiological risk is small and well below the AECB radiological risk criterion. The risk can be reduced through actions such as avoiding disposal sites containing known or suspected natural resources and locating the vault at its maximum practical depth. Another very effective action would be to provide redundant measures that extend the period of active and passive institutional controls. This last action could be very effective because, as shown in Figure 6-27, the peaks in the calculated risks occur relatively early in time.

7. LONG-TERM IMPACTS OF THE REFERENCE DISPOSAL SYSTEM

7.1 INTRODUCTION

The regulations specified by the AECB for an actual disposal system include criteria for times beyond 10^4 a. If the dose estimates do not reach their maxima within 10^4 a after closure, then reasoned arguments must be presented showing that (AECB 1987a)

- the rate of radionuclide release to the environment will not suddenly and dramatically increase,

- acute radiological risks (or acute doses) will not be encountered by individuals, and

- major impacts will not be imposed on the biosphere.

The results in Chapter 6 show that estimates of dose are increasing at 10^4 a (for the SYVAC scenarios) and, therefore, we evaluate potential impacts for longer time frames.

In this report, we focus on potential long-term impacts for an undisturbed disposal system. That is, we assume that the reference disposal system continues to function far into the future without being affected by any major disruptions. Our analysis includes consideration of the quantitative results for the SYVAC scenarios for times up to 10^5 a following closure of the reference disposal facility. We also provide reasoned arguments to evaluate impacts over even longer time-scales, provided no major disruptions occur. We then compare our results to the AECB criteria (AECB 1987a).

The EIS (AECL 1994a) provides more general discussions on potential effects of disruptions that could occur over long time frames.

7.2 PROJECTED TRENDS IN IMPACTS

7.2.1 Evaluation of Results to 10^5 a

As discussed in Section 5.8, the models and data used to describe the SYVAC scenarios can produce acceptable estimates of impact up to about 10^5 a following closure, provided that no major events occur during this period that would significantly disrupt or disturb the system being modelled.

The overall trends for the SYVAC scenarios show that estimated annual dose and risk are zero at earlier times and continue to increase for times up to 10^5 a (Section 6.5.2). During this entire time period, the estimated annual dose is many orders of magnitude below the annual dose associated with the AECB risk criterion, and even further below the total annual dose from naturally occurring sources of radiation. Moreover, the results in Sections 6.5.3 and 6.5.4 indicate that there would be no significant impacts on the biosphere, including any chemical toxicity effects or radiation doses to nonhuman biota, for times up to 10^5 a. This is the expected behaviour for a well-designed nuclear fuel waste disposal facility, which would provide protection from the radioactive material for long periods of time.

The analysis of the SYVAC scenarios shows that the estimated total annual dose for times up to 10^5 a is dominated by contributions from just two radionuclides: ^{14}C and ^{129}I. There are no significant contributions from all other radionuclides listed in Table 5-4. Carbon-14 and ^{129}I have four common characteristics that lead to this result; both radionuclides

- are relatively long-lived,
- have a significant inventory fraction that is instantly released from the used-fuel bundles (Section 5.2),
- are relatively abundant in used fuel, and
- are mobile in (or weakly sorbed by) media in the vault and in the rock surrounding the vault.

The discussion in Section 6.5.2 notes that the time of the maximum in the mean dose resulting from ^{14}C is about 4 x 10^4 a. (Because of parameter uncertainties, doses from ^{14}C will peak at different times in different simulations. However, the distribution of results for peak doses and time of peak doses are not the same. Thus the time of the maximum in the mean dose, about 4 x 10^4 a, is slightly smaller than the average of the times at which the peak doses occur, about 6.6 x 10^4 a.) Annual doses from ^{14}C reach a maximum relatively early, compared with ^{129}I, because ^{14}C has a half-life of only 5730 a. Carbon-14 is relatively mobile both in the vault and in the geosphere, but only small quantities survive its transport to the biosphere. For ^{14}C, the combination of its half-life, mobility and transport times to the biosphere result in decreases in the mean of estimated annual doses for times beyond about 4 x 10^4 a.

This result has implications for other radionuclides that have short half-lives and that are not renewed by ingrowth. (The following discussion would also apply to the initial inventories of progeny radionuclides but not necessarily to progeny inventories arising from subsequent ingrowth from its precursors in a decay chain.)

- Radionuclides with half-lives much shorter than ^{14}C, even if mobile in the buffer, backfill and rock, would not survive long enough to cause significant doses. For example, radionuclides such as ^{3}H, ^{39}Ar and ^{90}Sr, with half-lives of 12.4, 269 and 29.1 a respectively, did not contribute significantly to the total annual dose in any of the simulations to 10^5 a.

- The initial inventories of radionuclides with half-lives of about 5×10^3 a will decrease by a factor of more than a million after 10^5 a. If these radionuclides have not made a significant contribution to dose by 10^5 a, then their contributions for times after 10^5 a would likely be negligible. Thus no significant contributions are likely from ^{93}Mo (with a half-life of 3.5×10^3 a), ^{240}Pu (6.54×10^3 a) and the initial inventory of ^{226}Ra (1.6×10^3 a).

Hence our assessment indicates that radionuclides with half-lives of about 5×10^3 a or less would be of no concern at long times (except, possibly for progeny radionuclides).

In contrast, our assessment shows that ^{129}I, with a half-life of 1.57×10^7 a, would be expected to reach its global maximum annual dose some time after 10^5 a in the reference disposal system. However, internal doses from ^{129}I cannot normally lead to an acute risk to a member of the critical group (we assume an acute risk is associated with a likelihood of receiving an annual dose exceeding 1 Sv/a). This statement can be made independently of any discussion of the performance of the reference disposal system because of the way that ^{129}I behaves in the human body. Iodine-129 concentrates in the thyroid gland and can give an internal dose that is at most about 3.9×10^{-2} Sv/a (Zach and Sheppard 1992). This value would always be reduced by isotopic dilution with stable iodine that occurs naturally in groundwater and elsewhere in the environment (Davis et al. 1993). External doses are expected to be very small from a consideration of exposure pathways and the small amounts of ^{129}I that would discharge and remain in the vicinity of the critical group (see Figure D-34 of Appendix D). Accordingly, although the maximum annual dose from ^{129}I certainly occurs in the far future, the projected trends indicate that its maximum possible value would be far below the dose level associated with an acute risk.

Only one other radionuclide shares at least three of the four characteristics noted above for ^{14}C and ^{129}I. Krypton-81 has a long half-life (2.1×10^5 a), is instantly released from the used-fuel waste matrix and is mobile in the vault and geosphere. However, ^{81}Kr has a relatively small abundance in used fuel (Table 5-4). In addition, ^{81}Kr is generally of little concern because it is not retained in human tissue, and thus internal doses are extremely small. External doses (from sources in air) are usually most important for ^{81}Kr in safety assessments, but are of no consequence in the SYVAC scenarios because estimated concentrations of ^{81}Kr are effectively zero everywhere in the biosphere. Krypton-81 did not make a significant contribution to total annual dose in any of our simulations.

Krypton-85 is also assumed to be instantly released from the used-fuel matrix and is mobile in the vault and geosphere; moreover, it is almost 10^6 times more abundant than ^{81}Kr in used fuel (Table 5-4). However, ^{85}Kr has a short half-life (10.8 a), thus it does not survive long enough to produce a significant contribution to total dose in any of the simulations studied. Similar observations follow for two other radionuclides that are assumed to be instantly released and short-lived: ^{3}H and ^{39}Ar. Another instantly released radionuclide, ^{90}Sr, is both short-lived and immobile in the vault and the geosphere, thus it does not make significant contributions to estimated dose.

Six other radionuclides are assumed to have significant instant-release fractions from used fuel: ^{135}Cs (with a half-life of 2.3×10^6 a), ^{40}K ($1.28 \times x10^9$ a), ^{87}Rb (4.7×10^{10} a), ^{79}Se (6.5×10^4 a), ^{126}Sn (1.0×10^5 a) and ^{99}Tc (2.13×10^5 a). They are generally long-lived and relatively abundant in used fuel (Table 5-4). However, in all simulations to 10^5 a, none of these radionuclides produces significant maximum annual doses because they are relatively immobile in the natural and engineered media between the containers and biosphere (Section 6.4).

The previous paragraphs have considered all instantly released radionuclides: ^{39}Ar, ^{14}C, ^{135}Cs, ^{3}H, ^{129}I, ^{81}Kr, ^{85}Kr, ^{40}K, ^{87}Rb, ^{79}Se, ^{90}Sr, ^{99}Tc and ^{126}Sn. Most of the inventory of these radionuclides, and the complete inventory of all other radionuclides listed in Table 5-4, are released from the used-fuel and Zircaloy matrices through the congruent-release mechanism (Section 5.2 and Johnson et al. (1994b)). There are no significant contributions to total dose for times up to 10^5 a from any congruent releases for any radionuclide.

One important explanation for this result relates to the long-term stability of the used-fuel and Zircaloy matrices. (Other reasons include, for different radionuclides, half-life, abundance and mobility.) The results in Section 6.4 indicate that these two matrices are very effective barriers. For example, results from the median-value simulation (Sections 6.3, 6.4 and D.2) show that congruent releases from used fuel and Zircaloy are extremely small for times up to 10^5 a because of the very small solubilities of the matrices (1.55×10^{-7} mol/m^3 for the used-fuel matrix and 1.79×10^{-6} mol/m^3 for the Zircaloy matrix). At these solubility levels, only a minute fraction (6.2×10^{-9} for used fuel and 2.3×10^{-7} for Zircaloy) of the associated contaminant inventories are released over 10^5 a in the median-value simulation.

There is uncertainty in the solubilities of these two matrices, and the distributions are skewed (Johnson et al. 1994b) for use in the randomly sampled simulations. Most values are small, but a few are large, and their average solubilities are greater (about 7.5×10^{-4} mol/m^3 for the used-fuel matrix and 4.3×10^{-2} mol/m^3 for the Zircaloy matrix) than those observed in the median-value simulation. In turn, a larger average fraction of the two matrices would dissolve, releasing a larger average fraction of congruently released contaminants. Nonetheless, results from the randomly sampled simulations indicate that the two waste matrices are still very effective barriers: the average fraction of the matrix dissolved over 10^5 years would be less than (approximately) 10^{-4} for the used fuel and 10^{-2} for Zircaloy. In addition, the solubility estimates for uranium are expected to become smaller as a function of time because of the substantial reduction in alpha activity. The uranium solubilities estimated in SYVAC3-CC3 are based on relatively high assumed levels of alpha activity and significantly overestimate expected solubilities that would obtain at longer times when alpha activity is smaller (Johnson et al. 1994b and Section 5.8).

The effectiveness of the used fuel and Zircaloy matrices should continue long past 10^5 a because they would be located in a geochemical environment that is expected to persist for long time frames. Thus there would be no sudden and dramatic increase in the rates of release of radionuclides from the dissolution of these waste matrices.

7.2.2 Projections to Longer Times

It might be expected that simulations for the SYVAC scenarios, if carried out to long enough times after closure, would eventually produce large annual doses. This is not the case. Sets of 1000 simulations for all 68 radionuclides listed in Table 5-4 (Section 5.9) have been extended to 10^8 a to test this possibility. We then calculated the mean values of maximum estimated dose over this extended time-scale. (Note that these calculations are extended far beyond the period of acceptability of the models and data, and the results should not be interpreted as credible estimates of effects. However, the calculations do provide information on the mathematical behaviour of the system model, and show the solutions are well behaved.)

- The mean value of maximum estimated annual dose, totalled for all radionuclides, is always several orders of magnitude below 1 Sv/a, the dose associated with an acute risk.

- In fact, for most radionuclides, the calculated mean maximum dose is many orders of magnitude smaller than the total annual dose from radiation in the natural environment (about 3×10^{-3} Sv/a).

- The three radionuclides with largest mean values of maximum estimated annual dose, for times up to 10^8 a, are ^{222}Rn and ^{234}Th and ^{129}I; their mean values are approximately 100%, 10% and 1% of annual dose from background radiation.

Radon-222 and ^{234}Th are members of the 4n+2 decay chain (Table 5-4). In general, they are not products from a fission reactor but arise from the radioactive decay of ^{238}U. Radon-222 (a large component of natural background dose), ^{234}Th and other progeny of the 4n+2 decay chain would be found in far greater abundances, relative to the inventory of ^{238}U, in uranium ore deposits compared with nuclear fuel waste.

Other results from the simulations extended to 10^8 a show the dose-time curve has several peaks corresponding to the arrival at the biosphere of different radionuclides. For example, a peak from ^{129}I occurs near 2×10^6 a. Most other peaks occur at much longer times and are from radionuclides that have long half-lives and that are relatively immobile or from radionuclides that are short-lived members of an actinide decay chain (all such short-lived radionuclides have one or more immobile precursors and many are themselves immobile). This is the case for ^{222}Rn and ^{234}Th, relatively short-lived progeny of the ^{238}U decay chain; their peaks occur at 10^8 a for these extended simulations.

Long after the relatively rapid release of the instant contaminants, following corrosion of the containers, the vault inventory would be largely comprised of the long-lived radionuclides from the slowly dissolving used fuel and Zircaloy. The fuel matrix would retain most of the ^{238}U and its decay products and most of the other radionuclides originally found in the fuel, and the Zircaloy would retain most of its radioactive activation products. Table 7-1 shows inventories of long-lived isotopes at different times, calculated using the assumption that the radionuclides remain in place. After about 10^6 a, the inventory is largely dominated by uranium and its decay products.

At very long times, a waste disposal vault resembles a high-grade uranium ore deposit. Hence the behaviour of natural uranium deposits can serve as a useful analogue for the performance of the vault and the radionuclides it would contain. There are some differences in the amounts and types of radionuclides in used fuel and in a uranium ore deposit. For example, at 10^6 a, used fuel contains relatively large quantities of long-lived ^{237}Np and ^{242}Pu which have not yet disappeared because of decay, and relatively small quantities of decay products such as ^{230}Th, which are slowly increasing because of ingrowth. (In the discussion below on natural analogues, we expect that isotopes such as ^{242}Pu and ^{237}Np would be retained in the used-fuel matrix and released congruently with the slow dissolution of the used-fuel matrix. Because they have relatively small abundances, their concentrations in the disposal system would be relatively small compared with the concentration of ^{238}U.) In contrast, a uranium ore deposit would contain relatively small quantities of natural fission products and isotopes of plutonium (Fabryka-Martin 1993, Fabryka-Martin and Curtis 1993, Curtis et al. 1994), but (for most deposits) relatively large quantities of isotopes from the natural decay of ^{238}U.

For both used fuel and uranium ore deposits, however, long-term impacts would likely be dominated by ^{238}U and its decay products. From this point of view, it would be reasonable to expect that long-term environmental effects from the uranium in the disposal vault would lie somewhere in the range of environmental effects observed today from buried naturally occurring uranium ore deposits.

Studies have compared the potential health hazard presented by nuclear fuel waste, uranium ore and mine tailings (Mehta 1988; Mehta et al. 1991). The studies conclude that, ten years after discharge from a reactor, used fuel presents a health hazard (if ingested) about 100 times that of an uranium ore deposit containing the same amount of uranium. However, by 10^4 a, the hazard from the fuel has declined to the same order of magnitude as the ore deposit and remains thus thereafter (Mehta 1988; Mehta et al. 1991).

The long-term contribution to radiation in the natural environment by uranium in most uranium ore deposits arises mostly through the effects of its decay products, notably radioactive isotopes of radium and radon. These decay products tend to enhance radioactivity levels in local groundwaters and soil, and may lead to significant concentrations of radioactive radon

TABLE 7-1

RADIONUCLIDE INVENTORIES AT DIFFERENT TIMES*

Radio-nuclide	Source**	Half-Life*** [a]	Inventory [mol/kg(U)] at 0 a	10^4 a	10^6 a
^{10}Be	F	1.6×10^{6}	8.5×10^{-10}	8.5×10^{-10}	5.5×10^{-10}
^{10}Be	Z	1.6×10^{6}	1.7×10^{-10}	1.7×10^{-10}	1.1×10^{-10}
^{208}Bi	Z	3.68×10^{5}	9.7×10^{-14}	9.5×10^{-14}	1.5×10^{-14}
^{210m}Bi	Z	3.0×10^{6}	1.4×10^{-12}	1.4×10^{-12}	1.1×10^{-12}
^{14}C	F	5.73×10^{3}	1.8×10^{-5}	5.5×10^{-6}	0.0
^{14}C	Z	5.73×10^{3}	3.3×10^{-6}	9.8×10^{-7}	0.0
^{41}Ca	F	1.4×10^{5}	1.3×10^{-6}	1.2×10^{-6}	1.6×10^{-9}
^{135}Cs	F	2.3×10^{6}	1.8×10^{-4}	1.8×10^{-4}	1.3×10^{-4}
^{182}Hf	Z	9.0×10^{6}	2.2×10^{-8}	2.2×10^{-8}	2.0×10^{-8}
^{129}I	F	1.57×10^{7}	3.5×10^{-4}	3.5×10^{-4}	3.3×10^{-4}
^{40}K	F	1.28×10^{9}	2.2×10^{-7}	2.2×10^{-7}	2.2×10^{-7}
^{81}Kr	F	2.1×10^{5}	6.7×10^{-11}	6.5×10^{-11}	2.5×10^{-12}
^{94}Nb	Z	2.03×10^{4}	6.4×10^{-7}	4.5×10^{-7}	9.4×10^{-22}
^{59}Ni	F	7.5×10^{4}	3.6×10^{-6}	3.2×10^{-6}	3.4×10^{-10}
^{59}Ni	Z	7.5×10^{4}	1.0×10^{-6}	9.3×10^{-7}	9.9×10^{-11}
^{237}Np	4n+1	2.14×10^{6}	1.1×10^{-3}	1.1×10^{-3}	8.0×10^{-4}
^{231}Pa	4n+3	3.29×10^{4}	1.3×10^{-10}	9.0×10^{-8}	9.4×10^{-7}
^{205}Pb	Z	1.43×10^{7}	2.3×10^{-9}	2.3×10^{-9}	2.2×10^{-9}
^{107}Pd	F	6.5×10^{6}	5.1×10^{-4}	5.1×10^{-4}	4.6×10^{-4}
^{239}Pu	4n+3	2.41×10^{4}	1.2×10^{-2}	8.7×10^{-3}	7.5×10^{-15}
^{240}Pu	4n	6.54×10^{3}	4.3×10^{-3}	1.5×10^{-3}	2.8×10^{-13}
^{242}Pu	4n+2	3.76×10^{5}	2.5×10^{-4}	2.5×10^{-4}	4.0×10^{-5}
^{87}Rb	F	4.7×10^{10}	6.3×10^{-4}	6.3×10^{-4}	6.3×10^{-4}
^{187}Re	Z	5.0×10^{10}	2.7×10^{-6}	2.7×10^{-6}	2.7×10^{-6}
^{79}Se	F	6.5×10^{4}	1.6×10^{-5}	1.5×10^{-5}	3.8×10^{-10}
^{126}Sn	F	1.0×10^{5}	3.9×10^{-5}	3.7×10^{-5}	3.8×10^{-8}
^{99}Tc	F	2.13×10^{5}	2.1×10^{-3}	2.0×10^{-3}	8.0×10^{-5}
^{99}Tc	Z	2.13×10^{5}	2.6×10^{-8}	2.5×10^{-8}	1.0×10^{-9}
^{229}Th	4n+1	7.34×10^{3}	3.2×10^{-14}	5.4×10^{-8}	3.0×10^{-6}
^{230}Th	4n+2	7.7×10^{4}	5.5×10^{-9}	5.6×10^{-6}	7.3×10^{-5}
^{232}Th	4n	1.41×10^{10}	1.0×10^{-9}	1.5×10^{-6}	2.2×10^{-4}
^{233}U	4n+1	1.59×10^{5}	9.3×10^{-10}	3.4×10^{-6}	6.4×10^{-5}
^{234}U	4n+2	2.45×10^{5}	2.0×10^{-4}	2.0×10^{-4}	2.2×10^{-4}
^{235}U	4n+3	7.04×10^{8}	8.6×10^{-3}	1.2×10^{-2}	2.0×10^{-2}
^{236}U	4n	2.34×10^{7}	3.3×10^{-3}	6.1×10^{-3}	7.3×10^{-3}

continued...

TABLE 7-1 (concluded)

Radio-nuclide	Source*	Half-Life** [a]	Inventory [mol/kg(U)] at 0 a	10^4 a	10^6 a
^{238}U	4n+2	4.47×10^9	4.1×10^0	4.1×10^0	4.1×10^0
^{93}Zr	F	1.53×10^6	1.8×10^{-3}	1.8×10^{-3}	1.2×10^{-3}
^{93}Zr	Z	1.53×10^6	2.0×10^{-4}	2.0×10^{-4}	1.3×10^{-4}

* These data are calculated inventories of radionuclides with half-lives greater than 5×10^5 a and found in used-fuel bundles from a CANDU reactor. The data at zero years are the initial inventories reported in Table 5-4 and correspond to (median-value) inventories for bundles that have been out of the reactor for ten years. The inventories of most radionuclides decrease as a function of time because of radioactive decay. A few, such as ^{234}U and ^{230}Th, show an increase due to ingrowth from a precursor.

** Sources of the radionuclides are
- F - for fission products of UO_2 fuel or neutron activation products of fuel impurities;
- Z - for neutron activation products of Zircaloy materials; and
- 4n, 4n+1, 4n+2, and 4n+3 - for the four actinide decay chains.

*** Half-life data are taken from ICRP-38 (ICRP 1983).

in indoor air. Similar effects would be expected from the relatively large amount of uranium in the undisturbed disposal vault. The presence of the disposal system might cause a fractional increase in radioactivity in local groundwaters, owing to the slow release of long-lived ^{238}U and its progeny nuclides (with additional radioactivity from less abundant radionuclides such as ^{235}U, ^{237}Np and ^{242}Pu). Granite rock typically contains small quantities of uranium (Bowen 1979); for example, the granite of the Lac du Bonnet batholith contains about 7×10^{-3} grams of uranium per kilogram of rock (Gascoyne and Cramer 1987). Thus the mass of rock in the pluton containing the reference disposal vault could contain an amount of uranium exceeding the vault inventory and dominate the combined environmental effects resulting from the uranium in the rock and in the vault.

Natural high-grade uranium deposits are useful analogues, particularly if the uranium ore and associated radionuclides exist in an environment that has parallels with the reference disposal system. Natural analogue studies on deposits, such as those at Cigar Lake in Saskatchewan (Cramer 1986, 1994; Cramer and Smellie 1994; Goodwin et al. 1989) and Oklo in Gabon (CEC 1992; Berzero and D'Alessandro 1990; Brookins 1976, 1978, 1984; Cowan 1976, 1978; Curtis et al. 1989; Naudet 1978; Ruffenach 1978; Weinberg 1977), have provided valuable information related to many aspects of the disposal concept.

Our studies of the Cigar Lake deposit have focussed on particular aspects that have parallels with our reference disposal system. Most of the uranium ore at the Cigar Lake deposit is uraninite (Bruneton 1987), a uranium-IV oxide (mostly UO_2) whose composition is similar to that of used fuel. Studies at Cigar Lake indicate that uraninite (Cramer 1994)

- has been thermodynamically stable in the geochemical environment of the ore deposit,
- has remained in place for millions of years,
- has undergone extremely slow congruent dissolution, and
- has retained most of its nuclear reaction products (including products from spontaneous fission as well as decay products) with no significant movement for millions of years.

One of the more important reasons for these observations is connected with the geochemical environment found at the Cigar Lake deposit. The uraninite at Cigar Lake is located in an electrochemical environment that is naturally reducing and is surrounded by a clay-rich layer that has a low hydraulic conductivity (Cramer 1994). These conditions have close parallels with the conditions expected for a disposal vault located at depth in plutonic rock of the Canadian Shield. We expect an electrochemical environment in the disposal vault and surrounding geosphere that would be reducing and that would persist unless affected by a major disruption. We also expect that the engineered barriers, which include very low-permeability clay material in the buffer, would remain in place for times far beyond 10^5 a.

Similar results and conclusions are available from other analogues (Cramer 1994), such as the natural nuclear reactors found at Oklo. For example, a supporting observation from Oklo is the ability of uraninite to retain many of the fission products and activation products (notably isotopes of plutonium) for times of the order of two billion years in a system that is relatively open to groundwater movement (Brookins 1978, 1984; Cramer 1994; Curtis et al. 1989; Loss et al. 1989). Thus a comparison with natural analogues suggests that used fuel may persist for millions of years or longer, with slow congruent release of entrapped contaminants, so that projected impacts from the undisturbed reference disposal system would remain small or insignificant for long periods of time.

7.3 SUMMARY OF LONG-TERM IMPACTS

From these considerations for the reference disposal system, we conclude that no major impacts would be imposed on the biosphere, that the rate of radionuclide release would not increase suddenly and dramatically, and that radiation doses would be far below levels associated with acute doses or acute radiological risks.

The EIS (AECL 1994a) presents further reasoned arguments covering the potential effects of disturbances and disruptions to the disposal system such as evolution of the climate, glaciation, earthquakes, long-term releases of contaminants from the used-fuel matrix, the slow changes with time (or diagenesis) of buffer and backfill properties, human intrusion and meteorite impact.

8. SUMMARY AND CONCLUSIONS

8.1 INTRODUCTION

The previous sections describe the method used to assess the long-term safety of the disposal concept and demonstrate the application of the method to analyze qualitatively and quantitatively the impacts of a reference disposal system. In the following section, we compare the predicted impacts with the regulatory criteria and summarize the important features of the reference disposal system. We also examine how the results would be affected by recent information that has not been examined in depth in this assessment.

In Section 8.3, we indicate how the approach used in this postclosure assessment could be used for future studies of an actual disposal system. We also outline how results of the postclosure assessments could contribute to the decision-making process in future stages of a nuclear waste disposal program.

Finally, in Section 8.4, we put into context the results of our assessment and summarize the conclusions we believe are technically sound and defensible.

8.2 SUMMARY OF IMPACTS AND COMPARISON WITH REGULATORY CRITERIA

8.2.1 Summary of Estimated Radiological Risks

The AECB requires quantitative estimates of radiological risk to individuals in the critical group for times up to 10^4 a (AECB 1987a). For comparison with the AECB risk criterion, we must identify the scenarios that could contribute significantly to risk, and then estimate the probabilities of occurrence and radiation doses associated with each scenario.

1. For the reference disposal system, scenario analysis (Chapter 4) has identified three scenarios that require detailed quantitative evaluation to estimate their potential contributions to radiological risk for times up to 10^4 a. They are called the SYVAC, open-borehole and inadvertent human intrusion scenarios.

   The *SYVAC scenarios* describe groundwater-mediated processes that cause corrosion of the containers, release of contaminants from the nuclear fuel waste, movement of contaminants through the vault seals and surrounding rock, and eventual discharge of contaminants at the surface where they may result in environmental impacts. These scenarios are evaluated using the system model contained in SYVAC3-CC3, which contains a variety of switches to represent mutually exclusive factors (Chapter 4).

   The *open-borehole scenarios* describe an unlikely situation in which one or more open boreholes pass close to a vault room containing nuclear waste. An open borehole has the potential to by-pass the the massive geological barrier, and thereby contribute to the radiological risk of individuals in the critical group.

The *inadvertent human intrusion scenarios* describe a serious disruption of the integrity of the reference disposal system caused by a drilling operation that unknowingly takes place near the disposal vault some time after closure of the disposal facility. This drilling operation has the potential to cause the direct removal of nuclear waste from the disposal vault to the surface environment, and thus contribute to radiological risks of individuals in the critical group. The system model representing these scenarios estimates exposures to a member of the drilling crew, a technologist conducting drill-core examinations, a construction worker and a resident.

2. We have examined the probabilities of occurrence of these scenarios for use in the calculation of radiological risk.

We assume the sum of the probabilities of occurrence of the SYVAC scenarios is high, and we use a value of unity in our calculation of risk.

For the open-borehole scenarios, our detailed evaluation for the reference disposal system indicates that their probabilities of occurrence would be so small that they could not contribute significantly to the radiological risk (Section 6.7). Our conclusion is based on an evaluation of the effectiveness of three quality assurance procedures: one that ensures all boreholes are properly sealed, a second that locates any vault room containing nuclear waste beyond a minimum acceptable distance from any deep borehole, and a third that confirms there are no open boreholes near any vault rooms containing nuclear waste.

For the inadvertent human intrusion scenarios, we examine four cases in Section 6.8, drawing from the studies documented by Wuschke (1991, 1992). The probabilities of occurrence are very small, with maximum values that are less than 5×10^{-6} for all times up to 10^4 a. The probabilities also change with time because of considerations such as the length of time for which active and passive institutional controls are expected to be effective.

3. We have estimated the radiation dose associated with these scenarios, and (for the SYVAC and human intrusion scenarios) calculated the corresponding radiological risk. We use the risk equation specified by the AECB (1987a), with a modification (described in Section C.4 of Appendix C) when estimated annual doses exceed 1 Sv/a (the threshold assumed for deterministic effects on human health). The estimated dose and calculated risk pertain to a member of the critical group, a hypothetical group of individuals expected to receive the largest impacts from a disposal system. From the results discussed in Chapter 6, we reach the following conclusions.

For the SYVAC scenarios, our estimates of radiation dose have made use of both deterministic and probabilistic pathways analyses (Sections 6.3 to 6.6). The deterministic analysis is used to improve our understanding of the system model, whereas the probabilistic analysis is used to estimate impacts that include the effects of parameter uncertainty and variability. For the probabilistic analysis, the variable of interest is the arithmetic mean of a set of estimates of annual dose (AECB 1987a). We have calculated the arithmetic mean from sets of up to 40 000 randomly sampled simulations, and evaluated contributions from the 68 radionuclides (Table 5-4) found in the irradiated uranium dioxide fuel and Zircaloy sheaths from a CANDU reactor.

For the SYVAC scenarios, the arithmetic mean of the estimates of annual dose slowly rises to 1.0×10^{-11} Sv/a at 10^4 a after closure (Figure 6-18 and Section 6.5.2). The calculated radiological risk also rises slowly, to a value of 2×10^{-13} (chances of receiving a serious health effect per year) at 10^4 a. This radiological risk is more than 6 orders of magnitude smaller than the AECB risk limit of 10^{-6} serious health effects per year. Results from the median-value simulation show smaller values: the estimated annual dose at 10^4 a is 3×10^{-18} Sv/a (Section 6.3.2) and the probability of a serious health effect (risk) is 6×10^{-20} per year. The mean values from the randomly sampled simulations are considerably larger because of the effects of uncertainty, which produce a distribution of estimated impacts that is highly skewed. Most values are small, but a few are large, and the arithmetic mean dose is much greater than the corresponding estimate from the median-value simulation.

For the open-borehole scenarios, we noted above that their probability of occurrence is so small that these scenarios would not contribute significantly to the radiological risk (Section 6.7). Nevertheless, we have also estimated potential radiation doses associated with an open borehole that is deep enough to pass near the disposal vault. The results, discussed in Section 6.7.4, indicate that estimated annual doses attributed to an open borehole would be more than 4 orders of magnitude smaller than the dose associated with the AECB risk criterion, provided that there was a minimum distance of about 30 m between the borehole and any vault room containing nuclear waste. In fact, the actual minimum distance for the reference disposal system is likely to be much smaller than 30 m. We have also used SYVAC3-CC3 to simulate a situation where an open borehole passes just 5 m from a vault room containing nuclear waste, and the results suggest estimated annual doses would be less than the dose associated with the AECB criterion.

For the inadvertent human intrusion scenarios, estimated radiation doses are largest at earlier times and can exceed 1 Sv/a because these scenarios involve a by-pass of all protective barriers in the disposal system (Wuschke (1991, 1992) and Section 6.8). Their probabilities of occurrence are small near the time of vault closure, but tend to increase with time. From our analysis, we conclude that the calculated radiological risk reaches peak values of about 3×10^{-10} serious health effects per year within 300 a following closure of the disposal vault. This calculated risk is more than 3 orders of magnitude smaller than the AECB risk criterion. The results also indicate the radiological risk is decreasing at 10^4 a, because the rate of decrease in the estimated annual doses is greater than the rate of increase of probabilities of occurrence.

The *total radiological risk* is given by the sum of the risks from all significant scenarios; for the reference disposal system, the two significant scenarios are the SYVAC and inadvertent human intrusion scenarios. The resulting curve would be similar to that shown in Figure 6-27, because the calculated risk from the inadvertent human intrusion scenarios is much greater than the calculated risk from the SYVAC scenarios. Thus we conclude that, on the basis of our current understanding, the total risk is significantly smaller than the AECB risk criterion for all times up to 10^4 a. The discussion in Section E.2 indicates that this conclusion would remain unchanged when considering the 1990 revisions to the ICRP recommendations (ICRP 1991).

We conclude that the reference disposal facility would meet the radiological risk criterion of 10^{-6} serious health effects per year to individuals of the critical group for times up to 10^4 a, with a large margin of safety.

8.2.2 Summary of Estimated Chemical Toxicity Impacts

The AECB requires estimates of impacts associated with nonradioactive contaminants released from the disposal facility (AECB 1985, 1987a). Although we estimate chemical toxicity impacts only for the SYVAC scenarios (Section 6.5.3), we believe similar results and conclusions would apply to the other scenarios for the reference disposal system.

The analysis of the SYVAC scenarios includes simulations of the movement of nine chemical elements found in the nuclear waste: antimony, bromine, cadmium, cesium, chromium, molybdenum, samarium, selenium and technetium. The magnitude of their impacts generally depends on their concentrations in the water, soil and air used by members of the critical group.

Our study results show that bromine has the largest estimated concentrations in the local habitat of the critical group (Section 6.5.3). However, its concentrations are extremely small when compared with existing regulations and naturally occurring concentrations. For example, limits on bromine concentrations in water set by Health and Welfare Canada (1989) (see also McNeely et al. 1979) are approximately 10^{-3} mol/m^3. Our estimates of bromine concentration in well and lake water are more than 6 orders of magnitude smaller. Similarly, our estimates of bromine concentrations in soils near the discharge areas are also more than 6 orders of magnitude smaller than naturally occurring levels (Bowen (1979) reports a median concentration of bromine in soil of 1 x 10^{-4} mol/kg).

Estimated concentrations for the other eight chemically toxic elements are even smaller, and similar observations are made. Thus none of the nine chemically toxic elements deriving from the disposal vault would exceed existing regulations or guidelines, nor would they add significantly to the naturally occurring concentrations of these elements in the environment.

We conclude that the reference disposal facility would not lead to significant chemical toxicity impacts to individuals of the critical group for times up to 10^4 a.

8.2.3 Summary of Estimated Impacts on the Environment

The AECB (1987a) and the federal Environmental Assessment and Review Process Panel (EARP 1992) require that the disposal system provide for adequate protection of the environment from both radioactive and nonradioactive contaminants (AECB 1987a). We have carried out a detailed analysis of this topic for the SYVAC scenarios and believe that similar results and conclusions would apply to the other scenarios for the reference disposal system.

Our analysis of the reference disposal system for the SYVAC scenarios includes estimates of concentrations in the water, soil and air for the 68 radionuclides and 9 chemically toxic elements of concern (Section 6.5.4). These estimates pertain to that part of the environment that would potentially be most contaminated by the discharge of groundwaters that have passed through or near the reference disposal vault. The estimated concentrations are extremely small at all times, and hence we examine condensed results: the maximum (for times up to 10^5 a) of their mean estimated concentrations in the biosphere.

For each contaminant, we compare its maximum estimated concentrations with its environmental increments. Environmental increments are a measure of the variability in the baseline or existing concentrations of a contaminant in the environment, and they provide a stringent test to identify contaminants that are potentially significant (Amiro 1992a, 1993). Our comparisons show that only ^{14}C and ^{129}I have the potential to exceed their environmental increments for soil and water (Section 6.5.4). Thus only ^{129}I and ^{14}C in soil and in water require more investigation.

We have, therefore, examined further the potential effects of ^{14}C and ^{129}I. Our analysis shows that both ^{14}C and ^{129}I from the reference disposal vault would not lead to significant impacts on the environment for times up to 10^4 a. We base this conclusion on their possible chemical and radiological toxicity impacts. For instance, estimated annual doses to 10^5 a from ^{14}C and ^{129}I are many orders of magnitude smaller than the total annual dose from natural sources of radiation, for members of the critical group (Section 6.5.2) and for four nonhuman target organisms (Section 6.5.4).

Our studies indicate that the reference disposal facility would not lead to significant impacts on the environment for times up to 10^4 a, taking into consideration both humans and nonhumans that would reside in that part of the environment that would be most contaminated.

8.2.4 Summary of Impacts Beyond 10^4 a

If the dose estimates do not reach their maxima within 10^4 a after closure, then reasoned arguments must be presented showing that radionuclide releases to the environment will not suddenly and dramatically increase, that acute radiological risks will not be encountered by individuals, and that major impacts will not be imposed on the biosphere (AECB 1987a). Our analysis of the SYVAC scenarios for the reference disposal system shows that the estimated radiation dose is still increasing at 10^4 a and thus we have extended our studies to times beyond 10^4 a.

We consider quantitative arguments to the extent feasible, with additional support from qualitative arguments based on observational evidence and well-established scientific principles. The analysis in this report examines the projected behaviour of the reference disposal system, assuming it continues to operate far into the future without any major disruptions or disturbances. Additional documentation in the *EIS* (*AECL 1994a*) *discusses* the effects of potential disturbances.

Long-Term Behaviour of an Undisturbed Disposal System

The simulations performed for the SYVAC scenarios for times up to 10^5 a exhibit trends in contaminant transport and estimates of impact that would be expected for an undisturbed reference disposal system. The overall trends show that estimates of annual dose and risk are increasing for times up to 10^5 a (Section 6.5.2), although the estimated annual dose remains many orders of magnitude below the annual dose associated with the AECB risk criterion and even further below the total annual dose from naturally occurring sources of radiation. Thus acute radiological risks will not be encountered by individuals for times up to 10^5 a. The results also indicate that radionuclide releases to the environment will not suddenly and dramatically increase and that major impacts will not be imposed on the biosphere for times up to 10^5 a.

Projections to longer times (Section 7.2.2) indicate that doses from ^{129}I would become insignificant after about 10^6 a and that other radionuclides would eventually become important contributors to the total dose. After about 10^6 a, the inventory of radionuclides would be dominated by uranium and its decay products, and it would be appropriate to assess potential impacts through comparisons with impacts of naturally occurring uranium ore deposits. On this basis, we expect that no sudden and dramatic increases will occur in radionuclide releases to the environment, no acute risks will be encountered by individuals, and no major impacts will be imposed on the biosphere. These same conclusions are also reached when considering the effects of potential disruption and disturbances such as glaciation, earthquakes and meteorite impact (AECL 1994a).

We conclude that the reference disposal system will meet the requirements stated in the AECB Regulatory Document, R-104 (AECB 1987a), for times far into the future.

8.2.5 Important Features of the Reference Disposal System

We list here several important observations that follow from our analysis of the SYVAC scenarios for the reference disposal system.

- The deterministic analysis of the median-value simulation (Section 6.3) is useful both in describing the operation of the system model and in showing how the results can be related to specific features of the models and data. The probabilistic analysis (Section 6.5) is particularly useful because it includes the effects of parameter uncertainty and variability. These effects are clearly important; the results from randomly sampled simulations show a wide variation in possible impacts because of the underlying uncertainty in the model parameters. In addition, the estimated arithmetic averages of impacts from the probabilistic analysis are generally larger than the corresponding estimated impacts from the deterministic analysis because of this underlying uncertainty.

- Only two radionuclides (^{129}I and ^{14}C) and one chemically toxic element (bromine) reach the biosphere in appreciable quantities for times up to 10^5 a. These contaminants have several important characteristics in common: they are relatively abundant in the nuclear waste; they are released from the used-fuel bundles by the instant-release mechanism; they are very long-lived (bromine is not radioactive); and they are transported relatively quickly through the vault and geosphere because they are not strongly retarded by sorption processes or affected by precipitation. No other contaminant has more than two or three of these characteristics.

- An important element of the disposal concept is the use of multiple barriers (Section 6.4). For the disposal system analyzed in this assessment, important barriers include the titanium container, the used-fuel and Zircaloy waste matrices, the buffer and the backfill, the rock within the waste exclusion distance that isolates the vault from fracture zone LD1, and the remainder of the rock between the vault and the biosphere. These barriers act in concert; their combined effect is a multiplicative reduction in contaminant movement. Our analysis has shown that the effectiveness of a barrier is both nuclide-dependent and time-dependent and that all barriers contribute to the delay and attenuation of contaminant movement. Figure 8-1 shows the potential effectiveness of the reference disposal system for selected contaminants for times up to 10^5 a.

- Sensitivity analyses (Sections 6.3.3, 6.5.5, Sections D.5 to D.8 in Appendix D and Sections E.3 to E.7 in Appendix E) have identified a number of parameters that have a strong influence on estimated impacts. We studied one such parameter, the tortuosity of the lower rock zone, in some detail (Section E.7, Appendix E). Our parametric study shows how the tortuosity affects the magnitude of estimated annual dose and how the uncertainty in the tortuosity affects the magnitude and variability of estimated annual dose. These results and the corresponding results for other parameters can be used to guide future research studies. For example, our analysis indicates that it would be worthwhile to better quantify the tortuosity of the lower rock zone. More generally, because the tortuosity is interrelated with other parameters, we conclude it would be worthwhile to improve our understanding of contaminant transport in sparsely fractured rock.

- Sensitivity analyses have also helped to identify design constraints (Section 6.4) and to study site and design features (Section 6.6). Derived constraints are used to improve the expected performance and margin of safety of the reference disposal system. In defining the properties of the reference

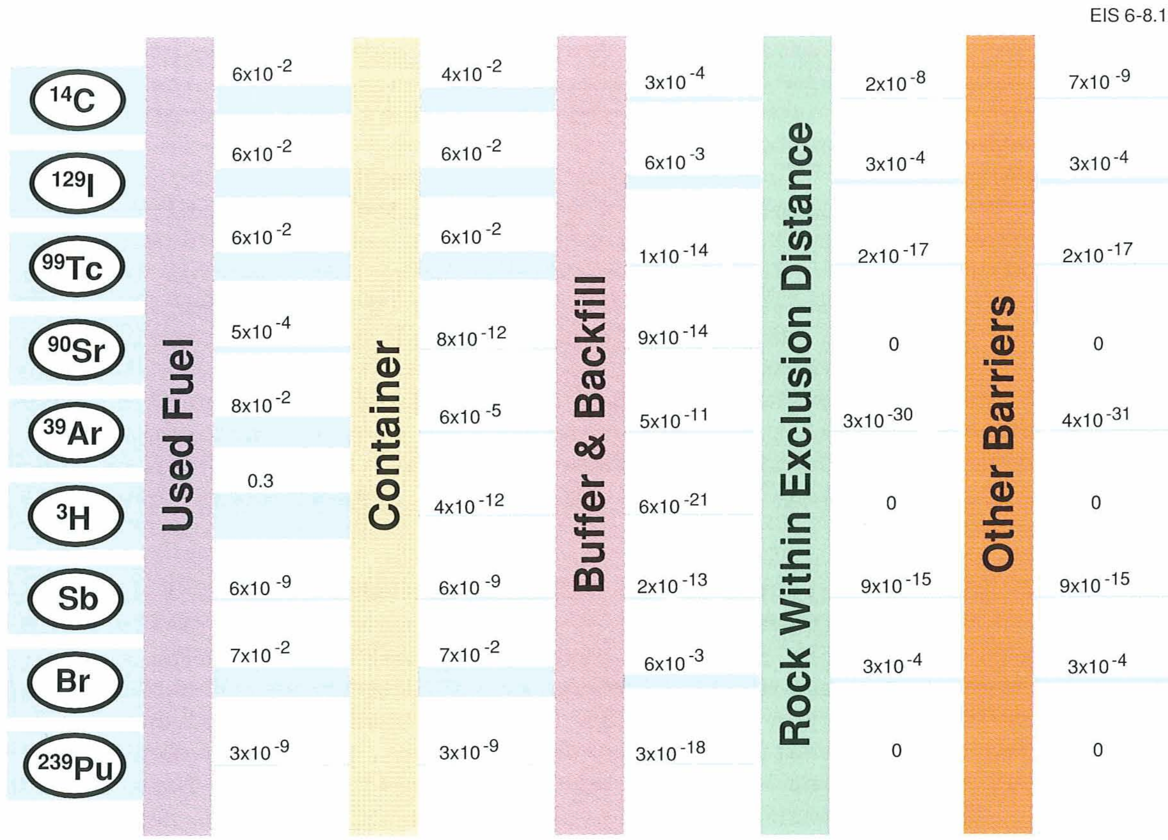

FIGURE 8-1: Barrier Effectiveness for Selected Contaminants.

These results show the effectiveness of several barriers for 9 contaminants, over a time-scale of 10^5 a. The 9 contaminants are identified on the far left, and the 5 vertical bars represent different barriers. The effectiveness of a barrier for a contaminant is shown by the change in widths of the horizontal shaded bars. (These widths are scaled logarithmically.) For example, the bar on the far left surrounding the label for ^{14}C represents a unit mass of ^{14}C placed in the used-fuel matrix at t = 0, and the bar leaving the "used-fuel" barrier shows the fraction that would escape over the next 10^5 a is only 6×10^{-2} or 6%. The remaining 94% has either decayed (to stable ^{14}N) or is still trapped in the used fuel. The fraction of ^{14}C that gets past all barriers is only 7×10^{-9}. Actually, this fraction would be much less than 7×10^{-9} because the method of calculation greatly overestimates effects of a sequential combination of barriers (Section 6.4).

The effectiveness of a barrier varies from one contaminant to the next. These results show the used-fuel matrix is very effective for ^{239}Pu and Sb but less so for the other contaminants; the underlying reasons are related to how contaminants are released from used fuel (Section 5.2 and Johnson et al. 1994b). More than one barrier may be very effective in controlling releases of a particular contaminant. For example, buffer and backfill, and rock within the exclusion distance, are very effective for ^{99}Tc.

disposal system, we selected a constraint pertaining to the orientation of the vault relative to a nearby fracture zone. When it is applied, this constraint improves the margin of safety by orders of magnitude and leads to considerably smaller estimates of radiation dose over times up to 10^5 a.

8.2.6 Effects of Recent R&D Information

The analysis presented here is based on an R&D program that has been in place for more than a decade. During this time, the models and data used in the postclosure assessment have steadily improved as more research results and information became available from our own research program, from similar programs in other countries, and from the general scientific literature.

In the following remarks, we discuss some recent information that could lead to significant changes in the models and data used in the postclosure assessment. We also describe the anticipated effects on the results and conclusions of this assessment.

- The ICRP has recently revised its recommendations for the calculation of dose and risk (ICRP 1991). The primary reference for the biosphere model (Davis et al. 1993) and a supporting document (Zach and Sheppard 1992) discuss these recommendations in more detail. Our analysis (Section E.2 in Appendix E) suggests that the revised recommendations would increase the estimates of annual dose by about a factor of 2 and risk by about a factor of 6. These small changes would not alter the overall conclusions of this postclosure assessment.

- Results from recent experiments suggest that some changes are required to the model describing the transport of contaminants in the vault, including diffusion in the buffer and the effects of transport across the buffer-backfill and backfill-rock interfaces. The changes, discussed in the primary reference for the vault model (Johnson et al. 1994b), would lead to small increases in the rates of release of ^{129}I and ^{14}C from the vault and to larger increases for ^{99}Tc. Scoping calculations using SYVAC3-CC3 suggest that corresponding increases would occur in the estimates of the total annual dose, principally from ^{129}I. However, the increases are so small that the overall conclusions of the postclosure assessment would remain unchanged.

- Other recent studies have suggested possible revisions to the data for the instant-release fractions for ^{14}C and ^{99}Tc. The new data would lead to much smaller instant releases of these two radionuclides (Johnson et al. 1994b) and would reduce their contributions to radiation dose. However, there would be little effect on total annual dose because neither ^{14}C nor ^{99}Tc are the major contributors to total dose.

- Recent information and work in progress at the WRA have identified a number of improvements to the network of segments used in the geosphere model and discussed in Section 5.4 and in the primary reference for the geosphere model (Davison et al. 1994b). In particular, current field information indicates that fracture zone LD1 does not extend down to or past the vault horizon and that LD1 is not hydraulically well-connected with other major fracture zones. Moreover, current field information indicates groundwater velocities in LD1 are smaller than those used in this report, and effects such as transverse diffusion (or diffusion into the rock matrix) may be significant (Davison et al. 1994b). We expect that these changes would lead to large decreases in contaminant transport and estimates of dose because of the importance of LD1 in the transport of contaminants from the vault to the biosphere for the reference disposal system. If the above improvements were implemented, the overall conclusions of this assessment would still hold, but the margin of safety would be much larger.

- Work is now in progress to improve our understanding and quantification of the long-term corrosion behaviour of titanium and other metals, such as copper. Research results indicate that these metals could be used to construct a very durable container (Johnson et al. 1994a,b). The analysis reported in Section 6.6 indicates that a such a container could be very effective in reducing impacts.

- This report has identified ^{14}C and ^{129}I as the main contributors to annual dose, and research is continuing to study their behaviour in the biosphere. Two studies of their rates of degassing from soils were completed in 1993.

  For ^{14}C, Sheppard et al. (1994) now recommend a rate constant that is about twice as large, but with a narrower range of possible values than the corresponding data used in this postclosure assessment. A larger rate constant would lead to increased degassing of ^{14}C, thereby reducing its concentration in soil and increasing its concentration in air. Given the relative importance of pathways involving soil and air, these new data might lead to smaller estimated doses attributed to ^{14}C. However, the average effect would be relatively small because the new data for the degassing of ^{14}C covers a narrower range (Sheppard et al. 1994).

  For ^{129}I, Sheppard et al. (in press) now recommend a rate constant that is about 33% smaller and that has a much smaller range of values than the corresponding data used in this postclosure assessment. A smaller rate constant for ^{129}I would reduce its rate of degassing, and thus would increase its estimated concentration in soil and decrease its estimated concentration in air. Because pathways involving soil are more important, slightly larger estimated doses from ^{129}I might occur. Nevertheless, the average effect is expected to be comparatively small because the new data for the degassing of ^{129}I covers a narrower range (Sheppard et al. in press).

- One potentially important radionuclide, ^{36}Cl, does not appear in Table 5-4 because Goodwin and Mehta (1994) concluded that it could not contribute significantly to the estimated dose because of its small inventory. However, this conclusion is being re-examined because recent information indicates that there are additional inventories (other than those reported by Tait et al. (1989)) of ^{36}Cl in irradiated CANDU fuel bundles. Studies are now in progress to better determine these additional inventories. Chlorine-36 is expected to behave much like ^{129}I in the disposal system, and bounding calculations suggest that radiation doses attributed to ^{36}Cl would be comparable to radiation doses resulting from ^{129}I. Thus the additional inventories of ^{36}Cl could increase the calculated radiological risk by a factor of about 2, but would not affect our overall conclusions.

8.3 POSTCLOSURE ASSESSMENTS OF OTHER DISPOSAL SYSTEMS

One objective of the postclosure assessment was to demonstrate an approach that can identify and estimate possible long-term environmental impacts when applied to a future implementation of the disposal concept.

Our approach is illustrated in Figure 2-1. The discussion in Chapter 2 shows how the approach can be used to integrate research information from many disciplines. The approach includes scenario analysis (Chapter 4) to identify the scenarios that require evaluation for a specific disposal system. We then show, for the reference disposal system, how a system model and associated data are constructed by drawing from a wide range of information (Chapter 5).

We demonstrate in Section 6.2 how preliminary analyses can be used to derive design constraints aimed at improving the margin of safety, and we use some of these design constraints to develop a final design for the reference disposal system. Sections 6.3 to 6.5 present a quantitative evaluation of the overall performance of this disposal system for thousands of years, including consideration of the effects of uncertainties, the effectiveness of individual barriers, and sensitivity analysis to identify important parameters and features. Our discussion in Sections 6.7 and 6.8 considers other scenarios whose probabilities of occurrence are expected to be small.

Finally, in Chapter 7, we show how potential impacts covering very long time-scales can be constructed from the quantitative results in Chapter 6, together with reasoned arguments and comparisons with natural analogues.

One strength of the approach is the inclusion of feedback processes. We have noted in previous sections that information generated in one step may necessitate a repeat of one or more previous steps. Thus the steps need not be completed in a strictly linear fashion because interim results of the analysis may affect subsequent planning and conclusions. Allowing for feedback is both a desirable and powerful feature of our assessment approach. It provides for incorporation of new research information as well as new information generated by the assessment itself. Using this approach, up-to-date information generated during the evaluation of any potential disposal site can be assimilated into preliminary assessments, and thus contribute to decision making in a timely fashion.

We believe the approach developed is sufficiently flexible that it could be applied by a future implementing organization to assess an actual disposal system based on the concept. In fact, we expect that the postclosure assessment would play an integral role in all stages of the implementation of a disposal system.

- During the siting stage, preliminary assessments would be performed for a number of different sites. Initially the models and data would be based mostly on reconnaissance studies, and the results would help to select a small number of sites for detailed investigation. For selected sites, more detailed information would become available from exploratory excavations, and would then be used to develop more detailed models and data. Subsequent postclosure assessments would contribute information, required as part of licensing actions, on the technical acceptability of each potential site, including information on how the performance of a site might be improved through the choice of particular engineering design features and the use of design constraints.

- During the construction of a disposal facility, further postclosure assessments would be performed, drawing from the large volume of information arising during construction. We expect that this information would lead to considerable refinement in the models and data because many of the assumptions made earlier will be resolved during the extensive characterization of the underground facilities. This large volume of research and field information would also provide increased confidence in the results of subsequent assessments. As the construction proceeds, results from preliminary assessments would contribute to the engineering design, with objectives aimed at improving both the cost-effectiveness and performance of the disposal system.

- During the operation stage, postclosure assessments would be used to confirm and refine operating and design constraints. Information from monitoring activities during and after operation will provide opportunities to further increase confidence in the models and data, and in the results of the assessments. Eventually, a "final" postclosure assessment would be completed, providing information important to the licensing decision to decommission and later close the disposal facility.

8.4 CONCLUSIONS FROM THE STUDY OF THE REFERENCE DISPOSAL SYSTEM

The models and data used in this report are based mostly on surface and limited borehole information, supplemented by research and development information on the environment and on a set of engineered system components. This information is roughly equivalent to what would be obtained during site evaluation prior to exploratory excavation.

The study has identified certain design and engineering constraints that would improve the margin of safety of the system that was analyzed, it has produced quantified estimates of impacts to the environment and to the hypothetical group of people who are most at risk, and it has identified components of the system that have the strongest influence on uncertainty in the estimates of impact.

The study results show that the estimated impacts for the reference disposal system are far below limits of regulatory requirements, even when uncertainties are taken into account. On the basis of expected conditions in the reference disposal system, it is reasonable to expect that the system would remain safe indefinitely into the future. Because the design used was not optimized for safety, and because many of the assumptions made tend to overestimate impacts, we believe that an optimized, well-engineered facility would provide an even greater margin of safety.

Finally, if the assessment pertained to an actual candidate site, these assessment results would support a decision to proceed with further exploratory studies, including exploratory excavation.

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APPENDIX A

METHODS OF ANALYSIS USED IN THE POSTCLOSURE ASSESSMENT

CONTENTS

A.1 INTRODUCTION

Several methods of analysis have been developed to implement the assessment approach described in the main text for the postclosure assessment. In this appendix, we give more detail on three such methods: scenario analysis, systems variability analysis (SVA) and sensitivity analysis. They are used in the six steps, shown in Figure A-1, to prepare the postclosure assessment.

Section A.2 describes scenario analysis (step 2 in Figure A-1). This tool was developed to identify the factors that must be included in assessing the future performance of a disposal system. It provides a systematic approach to provide confidence that all important factors have been weighed, with due concern for the time frame and specific objectives of the postclosure assessment. One of the outcomes of scenario analysis is the creation of a priority list of factors to be considered in the construction of mathematical models of the disposal system being studied.

Most of these factors are included in the SYVAC scenarios (Chapter 4 in the main text) for our study of the reference disposal system. They typically appear as parameters used in the mathematical description or system model. For instance, annual rainfall at a disposal site is described by a parameter that represents the long-term average. Related quantities can also appear in the model, such as the size of a lake near the disposal site and the size of the catchment area that drains into and through the lake.

The parameters used in the system model require numeric values, and these values may be uncertain. Experts must be consulted to determine whether a single value or a range of values is more appropriate. When a large number of parameters is described by different ranges of possible values, the assessment method may require special capability to deal with uncertainty. This is the situation we observe for the postclosure assessment.

Section A.3 describes the principal method used in this document for quantitative analysis of effects. Systems variability analysis, or probabilistic systems analysis, was developed to treat uncertainties in the parameters that define the mathematical model of a disposal system (Dormuth and Quick 1980) and is implemented in the SYVAC3-CC3 computer code. SYVAC3 is an acronym for <u>SY</u>stems <u>V</u>ariability <u>A</u>nalysis <u>C</u>ode, generation <u>3</u>; it is an "executive" code that performs SVA for any system model. Our assessment of the reference disposal system uses SYVAC3-CC3, where CC3 is an abbreviation of the models for the <u>C</u>anadian <u>C</u>oncept, version <u>3</u>, used to describe the reference disposal system. For the detailed quantitative studies described in this document, we use SYVAC3-CC3 in steps 3 through 5 of Figure A-1:

- Step 3 (develop models and data) produces computer models and parameter distributions to be used in estimating environmental impacts. We designed SYVAC3 to handle the types of models and parameter distributions needed for the assessment, including the "switch" parameters described in Chapter 4 in the main text. The use of SVA and SYVAC3 imposes some constraints on models and data; for example, the models should be computationally efficient so that thousands of simulations can be performed.

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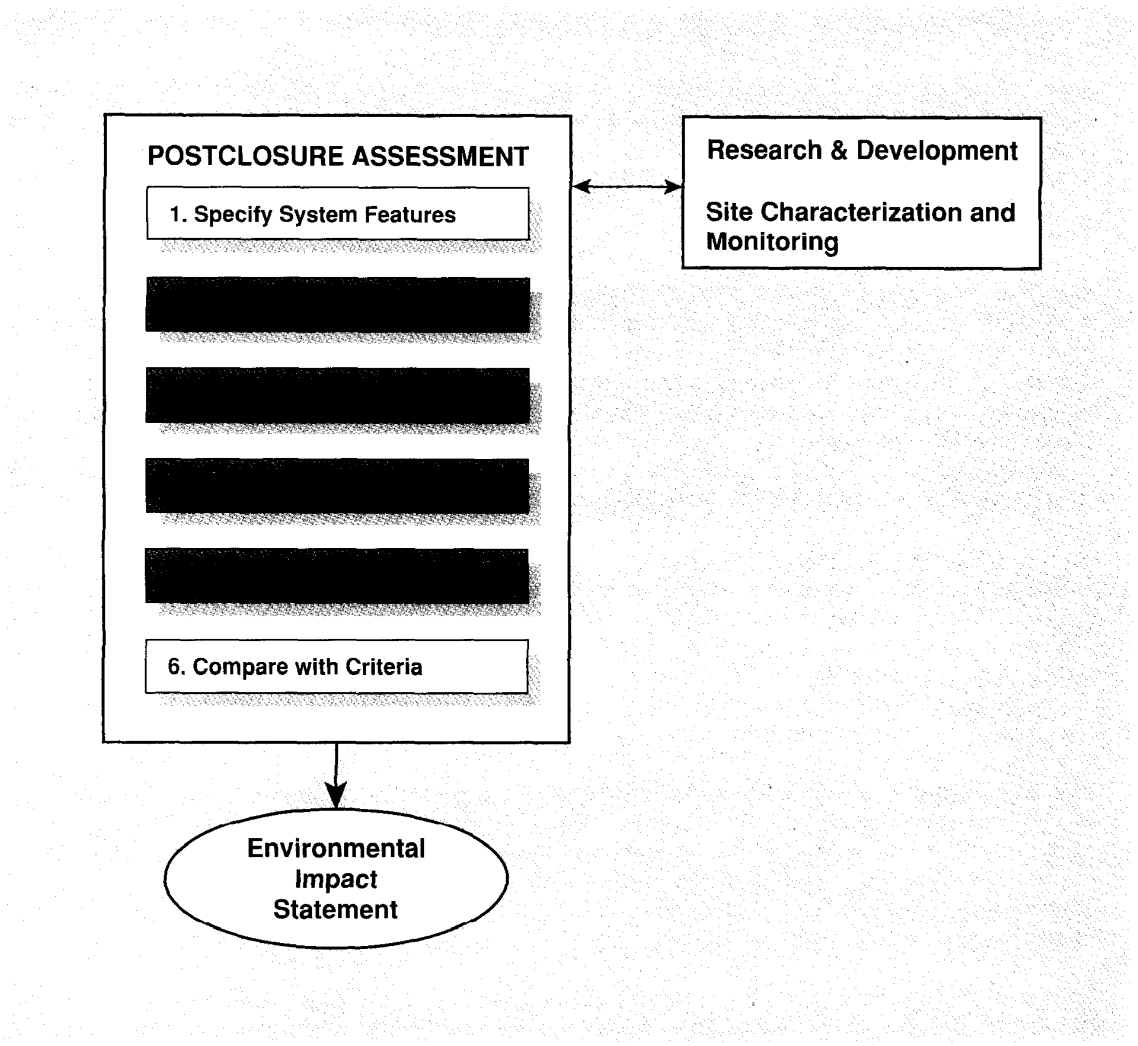

FIGURE A-1: Overview of the Six Steps in the Assessment Approach

Steps 2 through 5 use some special tools that have been developed for the postclosure assessment: scenario analysis, systems variability analysis and sensitivity analysis. These tools are described in Appendix A.

In applying this approach, the steps are not completed sequentially; instead, there is considerable feedback between steps. The figure also indicates that there exists a strong interplay between the postclosure assessment and the R&D program.

- In step 4 (estimate impacts), we perform thousands of simulations and complete enough simulations to obtain statistically robust estimates of important consequences. The number of simulations required depends not on the number of parameters in the system model but on their distributions. Consequences often have highly skewed distributions.

- Systems variability analysis simplifies step 5 (apply sensitivity analysis) by providing parameter distributions that can be used to define a common scale for variations in parameter values. For example, each parameter can be varied from its 10^{th} to its 90^{th} percentiles, so that the influences of different parameters are more readily compared. Systems variability analysis also generates large quantities of data from randomly sampled simulations that can be used in displaying the effects of important parameters.

Section A.4 documents our methods for sensitivity analysis. Sensitivity analysis is used to identify influential features of a mathematical model, and then to demonstrate how these features affect the model results. The complicated system model used in the postclosure assessment has a large number of parameters to analyze. At the same time, each simulation may require several minutes to run on modern computers. We have developed new methods to screen parameters and identify the influential ones using a small number of simulations. We apply sensitivity analysis to study variations for a single reference simulation (deterministic sensitivity analysis for the median-value simulation) and also for parameters varying across their full ranges (probabilistic sensitivity analysis).

Finally, in Section A.5, we outline our management of computer resources, and describe those resources, associated with running SYVAC3-CC3 and related computer codes.

A.2 SCENARIO ANALYSIS

A.2.1 INTRODUCTION

The postclosure assessment must estimate impacts for thousands of years into the future, and it is important to recognize and account for all possible long-term system characteristics that might lead to harmful long-term consequences. We must also identify issues that are likely to be important and ensure that they are accounted for in the assessment.

Several studies of important long-term safety issues were carried out during the course of the Canadian Nuclear Fuel Waste Management Program (CNFWMP) (Merrett and Gillespie 1983; Heinrich 1984a; Davis 1986a,b; Stephens et al. 1987; Stephens and Goodwin 1989). Scenario analysis is an evolution of these studies. It is a systematic procedure used to identify and describe all the important issues that should be examined in the postclosure assessment.

Scenario analysis has two main objectives:

1. Produce a comprehensive list of potential issues (factors) that could affect the operation of the disposal system. Scenario analysis provides a systematic approach to identify potentially important factors and gives confidence that all significant factors have been recognized.

2. Provide a logical framework for evaluating the importance of the factors. This framework leads to a set of scenarios, and all significant factors following from the first objective appear in one or more scenarios that require quantitative evaluation for times up to the first 10^4 a following closure of the disposal vault. Three scenarios are defined for the reference disposal system in Chapter 4 of the main text.

A factor is a distinguishing characteristic of the disposal system, its surroundings, or of perturbing external or internal events. Factors include features, events or processes that have the potential to affect some component of the disposal system, and thereby to affect the type or magnitude of the health and environmental impacts. Examples of these types of factors are

- features: vault geometry and layout, rock and buffer properties, presence of wells near the disposal site, surface water bodies, human diet;

- events: seal and grout failures, earthquakes, failure of dams, human intrusion into the vault after closure, agricultural fires, forest fires; and

- processes: container failure resulting from corrosion, chemical alteration of the vault buffer, diffusion of contaminants in pore water, weathering of rock, chemical interactions between contaminants and minerals, soil leaching, irrigation of crops.

A scenario is "a sketch, outline or description of an imagined situation or sequence of events" (NEA 1992) or, in the postclosure assessment, a possible future of the waste disposal site that takes into account a specified set of factors. These factors describe possible mechanisms affecting the performance of the disposal system in immobilizing and isolating nuclear fuel waste. Several scenarios may be defined, depending on the number of distinct combinations of factors that are feasible.

The following discussion summarizes the scenario-analysis procedure that was developed for the postclosure assessment (Goodwin et al. 1994). Its application to the reference disposal system studied in this postclosure assessment is summarized in Chapter 4 in the main text.

A.2.2 THE PROCEDURE FOR SCENARIO ANALYSIS

The procedure developed for scenario analysis is based on a scheme introduced at Sandia National Laboratories (Cranwell et al. 1982, 1987; Bonano et al. 1989). It also draws on work by the International Atomic Energy

Agency (IAEA 1985), the Swedish Nuclear Fuel and Waste Management Company (Andersson et al. 1989) and the Organization for Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA 1992).

The procedure for scenario analysis consists of the six steps shown in Figure A-2. The first three steps are focussed on the first objective of scenario analysis; they yield a comprehensive list of factors that could influence the performance of the disposal facility for a particular case study. The second three steps concentrate on the second objective; they yield a set of important scenarios that should be evaluated quantitatively. These steps should be completed by a group whose members encompass a wide range of expertise.

In the following paragraphs, we describe the six steps in the procedure, including some pragmatic recommendations resulting from its application. One such recommendation is especially notable: to make the procedure workable, the scope of the analysis should be restricted as early as possible. Thus in applying the first three steps, we focussed the analysis to the concept for disposal of Canada's nuclear fuel waste, which made the search for all potentially important factors more tractable. We further focussed the analysis, for steps three to six, on the reference disposal system evaluated in this document. The use of this particular (but hypothetical) disposal facility at a specific site has helped to develop a priority list of important factors and to identify scenarios requiring quantitative evaluation.

Step 1 - Identify Factors

The objective of the first step is to prepare a comprehensive list of factors. The list is obtained following a series of unconstrained, free-ranging meetings, with no restrictions on the types of factors identified. Other related studies also need to be reviewed, to help create an initial list of factors.

It is useful to limit the scope of this step to one particular concept for waste disposal because a formidable list of factors would be obtained when considering disparate concepts such as deep geological disposal and disposal in solar orbits.

Step 2 - Classify the Factors

The list of factors identified in step 1 are re-organized and re-ordered. Many different classification schemes are examined, with the objective being to identify missing factors.

Examples of classifications include

- type of factor: feature, event or process;
- component of the disposal system mostly affected: vault, geosphere or biosphere;
- subcomponents affected, such as the wasteform, container, buffer and backfill in the disposal vault;

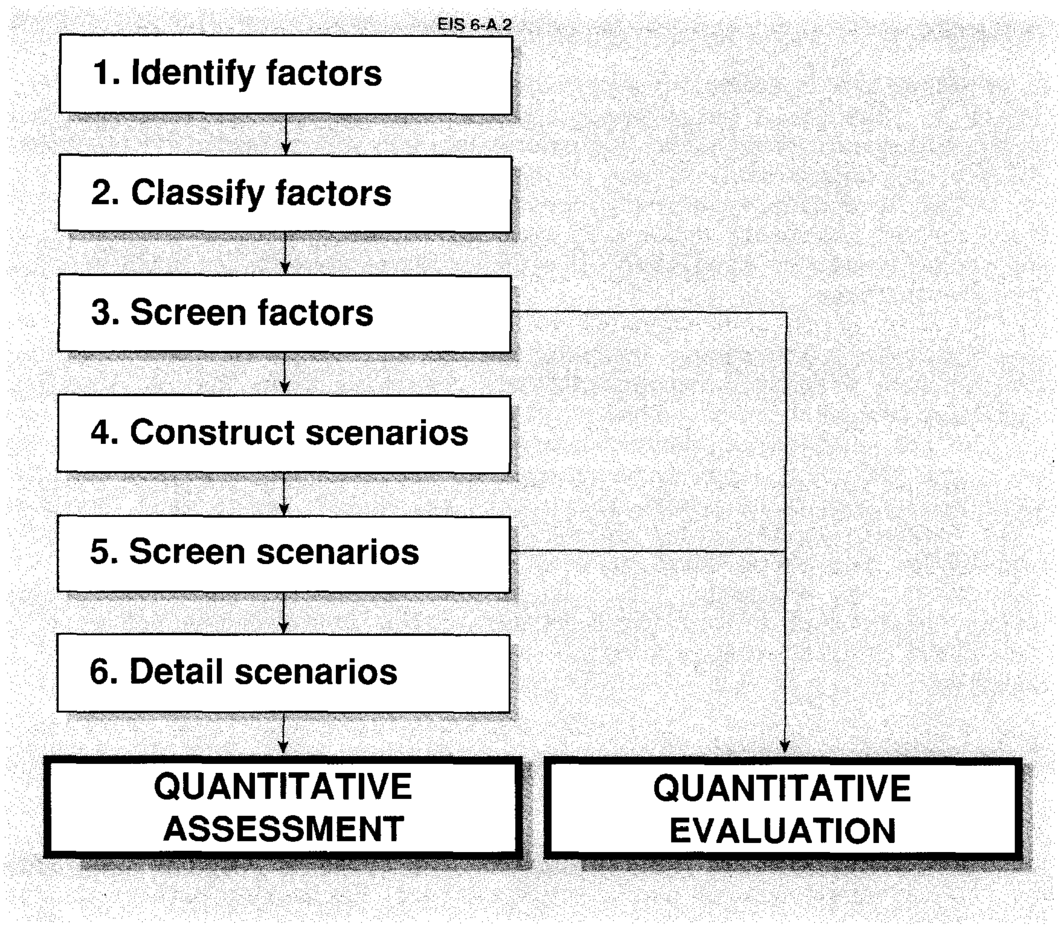

FIGURE A-2: The Six-Step Procedure Used to Identify and Select Scenarios for the Postclosure Assessment

The functions of the six steps are to

1. identify all the factors that might conceivably have an impact on the behaviour of the disposal system,
2. use various classification schemes to identify additional factors not identified in the first step,
3. screen the factors so as to create a priority list identifying those that require further evaluation,
4. integrate the factors from step 3 to form a complete set of scenarios,
5. review these scenarios to identify those that require further assessment, and
6. provide the descriptions required for subsequent mathematical modelling.

The scenarios described in step 6 are then subjected to further evaluation in the postclosure assessment. The procedure also requires evaluation of and justification for all factors and scenarios that have not passed the screening in steps 2 and 5.

- origin of the factor: naturally occurring, vault-induced, or human-induced;
- major mode of action: biological, chemical, or physical; and
- pathway by which the critical group would be affected: ingestion, inhalation or external exposure.

Step 3 - Screen the Factors

The purpose of step 3 is to examine each of the factors listed in the first two steps and to establish a priority list of important factors needing further evaluation. In fact, we established two priority lists: the first pertains to times up to 10^4 a, and the second extends to times beyond 10^4 a (reflecting regulatory criteria (AECB 1987), which proscribe how the postclosure assessment should address the two time frames). Important factors are passed onto step 4. The other factors are those considered sufficiently unimportant that they do not warrant further consideration.

This priority list can change for an assessment of a different disposal system or even for another assessment of the same disposal system. As more information becomes available, it may be feasible and important to add some factors to the list passed onto step 4. Conversely, assessment studies may indicate the deletion of some factors that had previously been passed. Our experience has been that the list tends to grow in size: new factors are added, but rarely are any factors deleted. Although some factors now known to be unimportant could be deleted for the analysis of the reference disposal system, they have invariably been retained because of the time and expense required to remove them from the computer code and data used in the postclosure assessment.

If a factor is not included in the priority lists, reasons for its elimination must be formally documented. Examples of such reasons might include

- A factor is considered to lie outside the scope of the assessment.
- Its probability of occurrence is so small that it could not contribute significantly to the risk associated with the disposal system.
- Its impacts are so small that it could not contribute significantly to the risk associated with the disposal system.
- It would not proceed to any significant degree or extent over the time frame of the assessment.

We strongly recommend that scenario analysis be focussed on a particular disposal facility at a particular disposal site as early as possible and, certainly, at or before this step in the procedure. In our experience, it is easier to develop credible arguments to justify elimination of many factors when dealing with a specific rather than a generic disposal system design and site.

Step 4 - Construct Scenarios

The goal in step 4 is to integrate systematically the important factors into a comprehensive set of scenarios that require further evaluation.

The recommended approach is to first define a central scenario that contains as many factors as possible. In general, the central scenario should include factors that are expected to be always important, that occur frequently, or that proceed to a significant degree over the time-scale of concern.

Our experience has been that the characteristics of the central scenario are strongly influenced by the approach available for subsequent estimates of impact, including the maturity of available models and data. We have also found that the flexibility offered by SVA (Section A.3) allows the combination of many simple scenarios into a compound scenario. They are combined by defining suitable "switch" parameters that control the selection of mutually exclusive options. For instance, Chapter 4 in the main text describes the SYVAC scenarios for the reference disposal system. This is the "central" scenario, and we refer to it in the plural to emphasize that these compound scenarios include many options, such as whether the source of drinking water for the critical group is a well or a lake. The corresponding switch parameter describes the probability of occurrence of the use of the well, and the thousands of simulations performed using SVA will sample the required number of simulations involving both options.

The remaining, or "residual" factors that do not appear in the central scenario are used to construct a complete set of alternative scenarios. For n residual factors, there are 2^{n-1} possible combinations containing one or more residual factors. Each alternative scenario then includes one of these combinations, plus all the factors appearing in the central scenario (except that any incompatible factors from the central scenario are excluded).

Our experience for the reference disposal system, discussed in Chapter 4 in the main text, has shown that some combinations of two or more low-probability residual factors would have extremely small probabilities of occurrence and need not be considered as scenarios. For example, the probabilities of occurrence near the disposal vault of a meteorite strike and a large earthquake are both very small, and there is no need to consider an alternative scenario involving an earthquake together with a meteorite (although there may be a need to examine separately an "earthquake" scenario and a "meteorite" scenario).

This approach can lead to a small number of scenarios passed on to step 5 if only a few factors are not included in the central scenario.

Step 5 - Screen the Scenarios

Each of the constructed scenarios from step 4 is reviewed to eliminate those judged not feasible or not important. As before, arguments must be documented supporting the elimination of a scenario. Examples of such arguments include those cited for step 3 and

- conservative estimates of impact may show that a scenario could not have a significant impact, and

- two or more similar scenarios can be combined into one scenario.

As in step 3, it is desirable to focus application of the procedure on a particular disposal facility at a particular disposal site because it is easier to develop credible arguments when the design and site are specific and not generic.

Step 6 - Define Scenarios

In the last step, the central scenario and any alternative scenarios are described in detail, to help guide the preparation of models and data for the postclosure assessment. The detailed descriptions identify important issues that require clarification, such as time duration and sequencing of factor effects.

A probability of occurrence is also assigned to each scenario requiring quantitative evaluation. In some instances this may not be feasible. For example, in applying the procedure to the reference disposal system, we concluded that it was not possible to assign in advance a credible probability of occurrence for the open-borehole scenarios (Chapter 4 in the main text): we expected that its probability of occurrence was small, but could not arrive at a quantitative statement. We resolved this problem by outlining a strategy describing how the open-borehole scenario should be handled in the assessment study. In effect, we postponed estimating the probability of occurrence of the open-borehole scenarios until the time of the detailed assessment. We could then draw on information from the analysis of the SYVAC scenarios to provide support for some of the discussion of the open-borehole scenarios.

A.3 SYSTEMS VARIABILITY ANALYSIS

A.3.1 INTRODUCTION

Scenario analysis (Section A.2) produces a list of factors that require quantitative evaluation in the postclosure assessment of the reference disposal system. Many of these factors appear as parameters in the associated mathematical description, or system model, of the reference disposal system.

We use the system model to estimate impacts and to compare these impacts with regulatory criteria. One of the more important criteria is the radiological risk limit set by the Atomic Energy Control Board (AECB) (1987), which must be met for 10^4 a following closure of the disposal facility.

Over this time-scale, much uncertainty exists in the values of many of the parameters used by the system model. The available data and understanding of the disposal system are limited to studies of short duration and limited ranges of experimental conditions. The assessment studies must extrapolate the data and understanding to chemical and physical conditions and to time-scales that are not directly accessible through laboratory and field studies. It is essential, therefore, that the assessment accounts for the uncertainty inherent in making such extrapolations.

There are several potential approaches for handling uncertainty in environmental impact assessment (see, for example, ERL 1985). For preparing quantitative estimates of impact for the postclosure assessment, the approach chosen is SVA (Dormuth and Quick 1980).

Systems variability analysis, more commonly known as probabilistic systems analysis, has matured considerably over the past two decades (Goodwin 1989a,b; Saltelli 1989). In particular, considerable progress in probabilistic systems analysis has been made by members of the Probabilistic Systems Assessment Code User Group (PSAC), organized in 1985 by the Nuclear Energy Agency (NEA) of the OECD, to develop and apply the SVA technique (Thompson et al. 1989). One important achievement of PSAC has been the completion of four international comparisons of codes implementing the SVA approach (PSAC 1987, 1989, 1990, 1993). As a founding member of PSAC, AECL has participated in PSAC activities and has benefited significantly from the exchange of information and ideas with other members of PSAC.

In the remainder of this appendix, we describe the SVA technique and provide some details on SYVAC3, a computer code that implements SVA and that has been used extensively in the postclosure assessment.

A.3.2 DESCRIPTION OF SYSTEMS VARIABILITY ANALYSIS

Systems variability analysis was developed to accomplish the following objectives:

- Assess a complex environmental system. A systems approach is required to describe all the important components of an environmental system, particularly when there is a complex interplay between components. A systems approach provides the means to evaluate the effectiveness of each component and the means to assess the system as a whole. Results from preliminary assessment studies can be used to focus detailed research on those components having the greatest influence on estimated impacts. Section 6.2 in the main text describes such a case, where we investigate derived constraints that could improve the margin of safety of the reference disposal system analyzed in this report. Later assessment studies can then help to optimize the system in terms of safety and cost.

- Account for the implications of our imprecise understanding of chemical, physical and biological processes that could affect the performance of the system. For the postclosure assessment, the effects of uncertainty and variability must be taken into account so that we can extrapolate current data and models into the distant future and describe conditions not directly accessible in laboratory and field studies.

These two objectives of SVA conform with the regulatory requirements for the postclosure assessment. A systems approach is appropriate because the radiological risk criterion (AECB 1987) is a measure of the performance of the entire disposal system. There are also requirements to account for uncertainty and variability when they affect the estimates of risk (AECB 1987).

Figure A-3 illustrates the SVA approach used in the postclosure assessment. It consists of two stages:

1. development of models and data, and

2. estimation of impacts.

The development of models and data is indicated schematically on the left-hand side of Figure A-3. Information is obtained from research in the laboratory and field, from detailed analysis of experimental and theoretical data and from the knowledge of experts. This information is used to construct a system model: the figure shows a system model that is a chain of three submodels representing the vault, the geosphere and the biosphere.

The information is also used to define the data required by parameters of the system model. A key feature of the SVA is the use of probability density functions (PDFs) for independent parameters. Thus the data for a parameter need not be limited to a single value; instead, it may span a range of values with different weights accorded to its possible values. Figure A-4 shows a sample PDF. There are two mathematical requirements of any PDF:

- the probability of any value must be greater than or equal to zero, and

- the integrated probability (the area under the curve in Figure A-4) must be equal to unity.

Some other special requirements of models and data are discussed below.

The second stage of the SVA approach, estimation of impacts, is illustrated in the box on the right-hand side of Figure A-3. A set of parameter values is sampled from their distributions and passed to the system model. The system model simulates the movement of contaminants through the vault, geosphere and biosphere, and produces an estimated impact, such as a set of radiation doses or chemical toxicity effects at selected times. The sampling, simulation and estimation of impact are repeated, using new sets of parameter values selected from their distributions. Typically, there may be a thousand or more repetitions, yielding as many estimates of impact. (The number of repetitions required for convergence of results is discussed in Section A.3.5.)

Each estimate of impact can be individually compared with regulatory criteria if desired. We can regard the thousand simulations as a thousand "what-if" assessments, in which each impact estimate corresponds to a particular combination of parameter values. We could then compare each annual dose estimate (ADE) with a corresponding criterion on radiological impact.

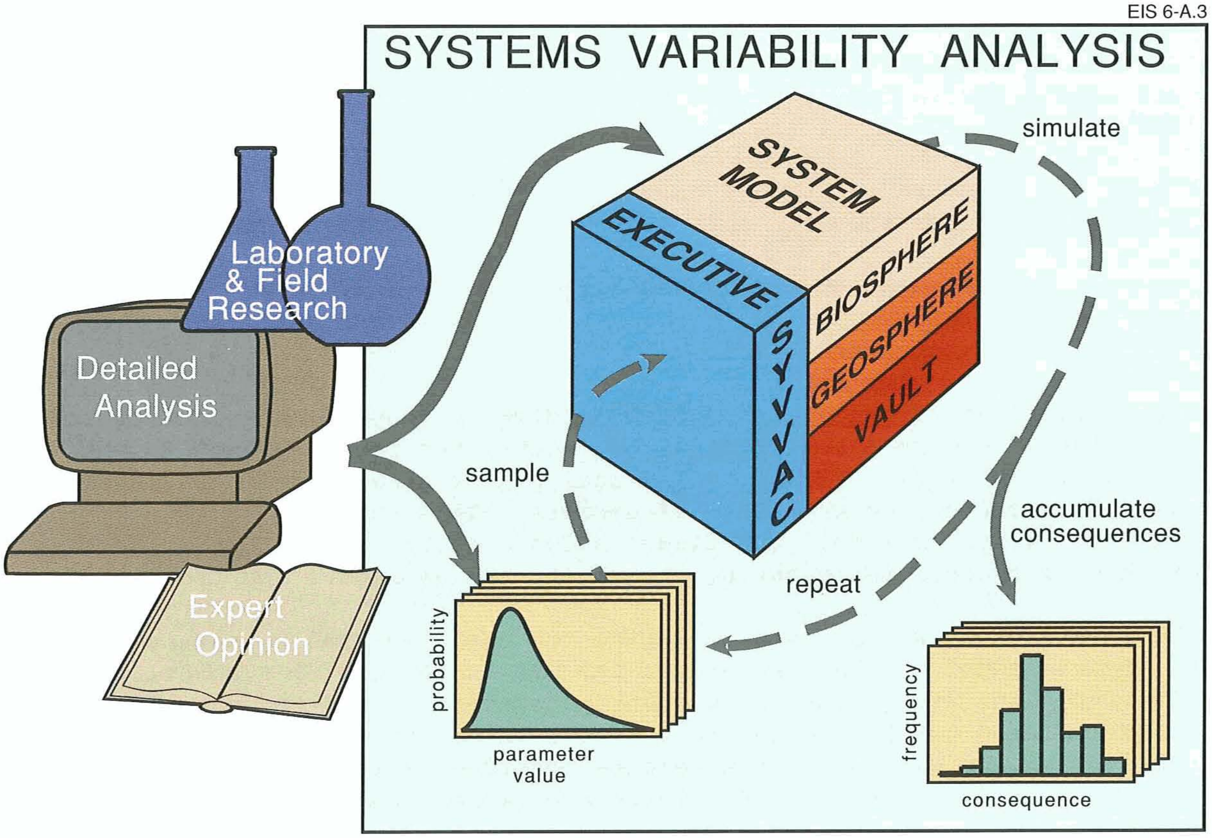

FIGURE A-3: Illustration of the Systems Variability Analysis Approach

Systems variability analysis (SVA) is a central tool used to prepare quantitative estimates of impact in this postclosure assessment. Models and data are developed from laboratory and field research, detailed analysis and expert opinion. The system model illustrated is composed of submodels representing the vault, the geosphere and the biosphere. The feasible values (and their likelihoods of occurrence) of a parameter in the system model are shown as a probability density function (PDF): a key feature of SVA is its ability to accept a range of possible values for each parameter, specified using different PDFs. A set of values for all the parameters in the system model is randomly selected from the appropriate PDFs. These values are then used in the system model to simulate the system and to estimate an impact. The sampling, simulation and estimation steps can be repeated many times to build up a set of impacts that reflect the underlying uncertainty in the system parameters. The SVA approach is implemented for the postclosure assessment in SYVAC, an acronym for SYstems Variability Analysis Code.

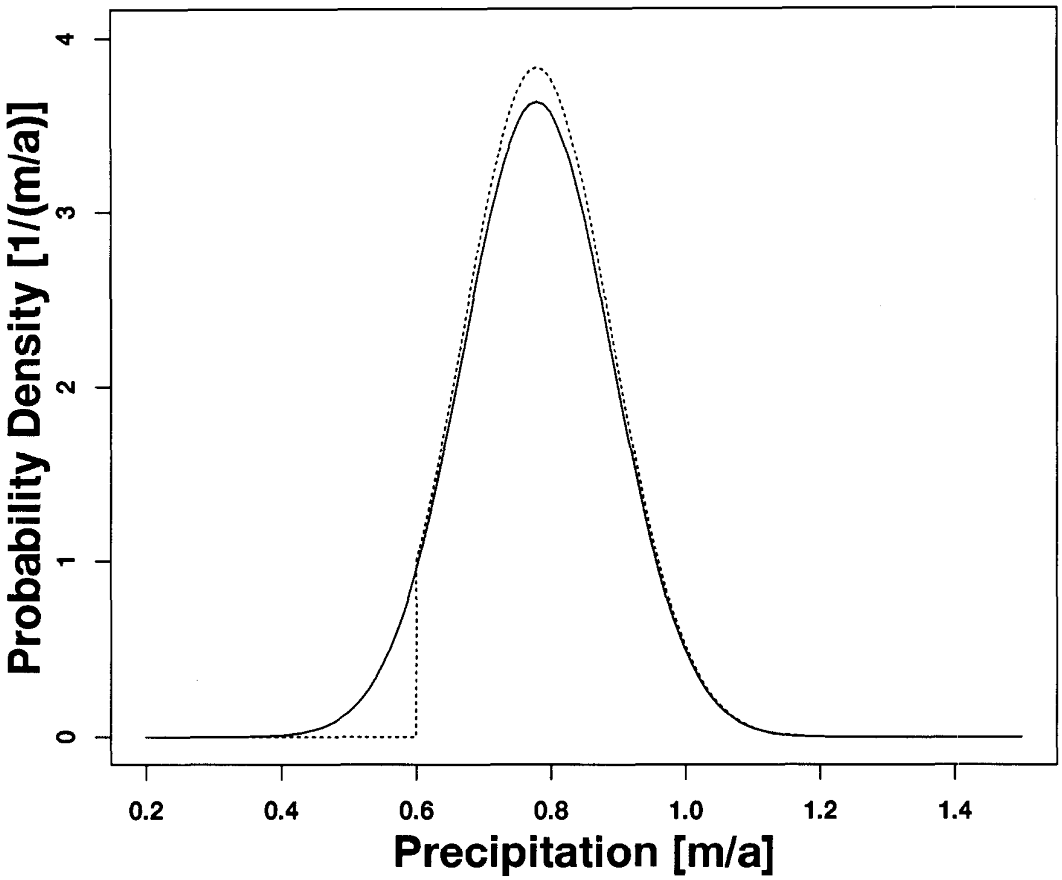

FIGURE A-4: Example of a Probability Density Function

The solid line shows the PDF for the net annual precipitation (Davis et al. 1993). It is a normal PDF with a mean and standard deviation equal to 0.78 and 0.11 m/a respectively, and with a lower bound of 0.20 m/a (although this has no noticeable effect in the plot). The dotted line illustrates the effect of truncation at 0.6 m/a; the probability density is then zero at values less than 0.6 m/a and is increased elsewhere, such that the integral of the (truncated) PDF remains equal to unity.

Alternatively, all estimated impacts can be combined. Figure A-3 shows a histogram for an estimated impact versus its frequency of occurrence. In this sample histogram, the estimated impact could be a combination of all radiation doses at some time, or it could be the maximum concentration in time of a chemically toxic element at some position in the biosphere. The distribution of impacts reveals the underlying uncertainty in the model parameters, as captured by the thousand simulations. Another important combination is possible if the parameter values are randomly sampled from their distributions. The average of the estimated impacts corresponds to the statistical expectation value of the calculated impact. This expectation value can be compared with the regulatory guidelines, standards and criteria, with the advantage that the underlying uncertainty in model parameters is folded into the estimate. With random sampling, it is also possible to calculate the statistical confidence level of the estimate of expected impact (Andres 1986, 1987; see also Section A.3.5).

The SVA approach followed for the postclosure assessment, therefore, reflects the overall performance of the entire disposal system and accounts for uncertainty and variability in the parameters that define the system model.

The successful application of SVA depends strongly on the quality and characteristics of its system model and data. Five important requirements of models and data are the following:

- The system model and data must be capable of extrapolation, to cover long periods of time or chemical and physical conditions that cannot be studied in the laboratory. This requirement may be a controlling factor in the selection of the model and its associated data. For the postclosure assessment, we have frequently made conservative assumptions in developing the system and data, such that subsequent extrapolations are defensible (Johnson et al. 1994, Davison et al. 1994, Davis et al. 1993).

- Because the system model and data must take into account uncertainty and variability, it may limit the choice of the model and associated data. For the postclosure assessment, a set of general guidelines was available to define PDFs for the model parameters (Stephens et al. 1989, 1993).

- The system model must be sufficiently comprehensive to describe all the important components of the system and yet simple enough to perform thousands of simulations in a reasonable time. For simulations using a computer, there is an extension: the computer code must be numerically stable (or robust) so that it can correctly deal with thousands of different combinations of parameter values.

- The data must take parameter correlations into account. The SVA approach may generate thousands of sets of sampled parameter values, and it is important to ensure that the combination of parameter values within every simulation is physically possible. Parameter correlations are taken into account in the postclosure assessment; for instance, there is a correlation between the amounts of food and water consumed by members of the critical group to ensure that values chosen for these two parameters are consistent.

- The models and data used must be of high quality because they underpin the reliability of the postclosure assessment. Model evaluation (compare with model validation, Appendix B, Section B.2) checks whether the phenomena controlling the impacts are adequately represented, and evaluation support for the models and data is provided in the primary references on the vault model (Johnson et al. 1994), the geosphere model (Davison et al. 1994) and the biosphere model (Davis et al. 1993). Verification tests the implementations of the models against alternative implementations and ensures that the data are consistent with its source; it also checks whether computations using the models and data correspond to the mathematical expression of the models.

Verification support, discussed in Appendix B, describes the detailed code and data checks and software quality assurance program for the computer code SYVAC3-CC3.

The computer code SYVAC3-CC3 implements the SVA approach for the postclosure assessment. It is described in more detail in the next section.

A.3.3 DESCRIPTION OF SYVAC3-CC3

The system model for the postclosure assessment, describing the high-probability situation called the "SYVAC" scenarios, is complex. It requires a large number of parameters to describe the expected performance of the disposal system for the 68 radionuclides and nine chemically toxic elements evaluated in this document. Chapter 5 in the main text describes the more important parameters, and Szekely et al. (in preparation) list all parameters and their values used in this assessment.

To handle this complex model, we have developed a host computer code called SYVAC3 (Goodwin et al. 1987a). The SYVAC3 code directs the second stage of the SVA approach; that is, it controls the sampling and simulation, and produces a set of corresponding estimates of impact.

The SYVAC3 code is not a complete computer code; it must be linked with a mathematical model that describes the system to be analyzed. For the postclosure assessment, this system describes the reference disposal system, a hypothetical implementation of the concept for disposal of Canada's nuclear fuel waste. The complete computer code is called SYVAC3-CC3. The contents of CC3 are fully documented in the primary references on the vault model (Johnson et al. 1994), the geosphere model (Davison et al. 1994) and the biosphere model (Davis et al. 1993) and are outlined in Chapter 5 in the main text of this report.

The SYVAC3-CC3 model uses more than 7000 parameters that are associated with the model of the reference disposal system. Many of these parameters are not required for all simulations or do not change for different simulations:

- For more efficient analysis, we have separated the contaminants identified in Section 5.9 in the main text into 11 groups, each containing seven to ten contaminants. One set of randomly sampled simulations may, therefore, involve only seven contaminants. Many of the parameters in the system model are contaminant-specific, such as retardation factors, plant/soil concentration ratios, thermodynamic equilibrium constants and radioactive half-lives, which may be different for different chemical elements or radionuclides. For a group containing ten contaminants, SYVAC3-CC3 requires only about 4000 parameters.

- Of these 4000 parameters, approximately 2600 are described using a "constant" PDF; that is, their values are the same in all simulations. They include the coordinates of the nodes for the network of segments in the geosphere and the number of chemical species appearing in a molecular formula. The remaining 1400 parameters are described using other classes of PDFs, such as normal, lognormal and uniform PDFs. Thus only about 1400 parameters vary from one simulation to the next in a set of random simulations.

SYVAC3 manages the simulation procedure of SVA. Figure A-5 shows the five basic functions of SYVAC3, which are to

1. Input Data for Model Parameters. This function is executed once every time SYVAC3 is run. SYVAC3 provides a facility to automate the assignment of model-specific data to the corresponding model-specific parameters.

2. Sample Parameter Values. For each simulation, a set of values is required for all the parameters that appear in the system model. The SYVAC3 code may be used to sample values for the following types of PDFs: normal, lognormal, correlated normal, correlated lognormal, uniform, log uniform, piecewise uniform, triangular and beta (Goodwin et al. 1987a). Figure A-6 shows examples of these functions. Two different sampling strategies are most frequently used in the postclosure assessment. For estimating arithmetic averages of impacts, we use random sampling (or Monte Carlo sampling). (To choose a random value, we use a random number generator to select a value between 0 and 1; this value is then transformed using the inverse cumulative distribution method (Knuth 1969, Rubinstein 1981) to the corresponding parameter value from its PDF.) For sensitivity analysis, we typically use parameter values that are fixed at prescribed quantiles of their PDFs, such as the 0.01, 0.5 and 0.99 quantiles. The SYVAC3 code may also be used to carry out deterministic simulations using selected values, such as the median value of every PDF.

3. Simulate System. For each simulation, the sampled parameter values are used in the system model to simulate the performance of the system.

4. Save Simulation Results. Specified results from each simulation can be saved in an auxiliary computer file. In SYVAC3-CC3, the results saved are all estimated impacts, values of important intermediate variables and values of all sampled parameters. These results are then available for subsequent analysis, such as plotting and statistical analysis.

5. Output Case Summary. The SYVAC3 code keeps track of each simulation and writes an overall summary of the results from each set of simulations. In SYVAC3-CC3, the summary records the number of simulations performed and the number successfully completed. It also records the number of simulations, if any, that require further examination because errors were detected.

Figure A-5 also itemizes a special function provided by SYVAC3. In Figure A-5, the bottom box "Time-Series Routines" provides numerical algorithms to handle time series, defined to be sets of ordered pairs, each consisting of a time value and the corresponding value of a variable. These routines are used extensively within SYVAC3-CC3 to represent all

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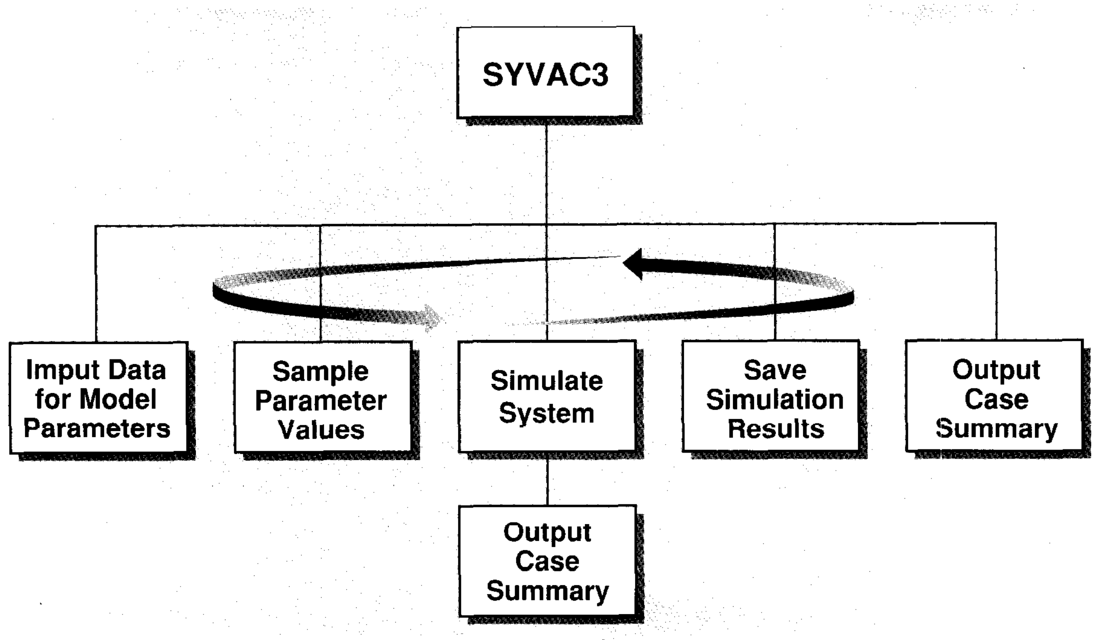

FIGURE A-5: Basic Functions of SYVAC3, Displayed as a Structural Hierarchy

The functions "Input Data for Model Parameters" and "Output Case Summary" are each executed once for a set of simulations. "Sample Parameter Values," "Simulate System" and "Save Simulation Results" are each executed many times, once for each simulation, as indicated by the looping arrow. The bottom box, "Time Series-Routines" represents a set of routines, provided by SYVAC3, that can be referenced by the system model during the simulation of the system.

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calculated variables that are a function of time, such as the rate of failure of containers, the flow of contaminants along a fracture, and the estimated annual dose. Chapter 6 in the main text contains many examples of plots of time series. Routines are available to perform many operations on time series, including add, multiply and convolve time series. The time-series routines can use an automatic selection of time steps to achieve a specified numerical accuracy in each time-series operation.

The time-series routines are also used in combination with routines from a mathematical algorithm library to solve systems of differential and partial differential equations used in the models (Heinrich 1984b, Heinrich and Andres 1985, LeNeveu 1987).

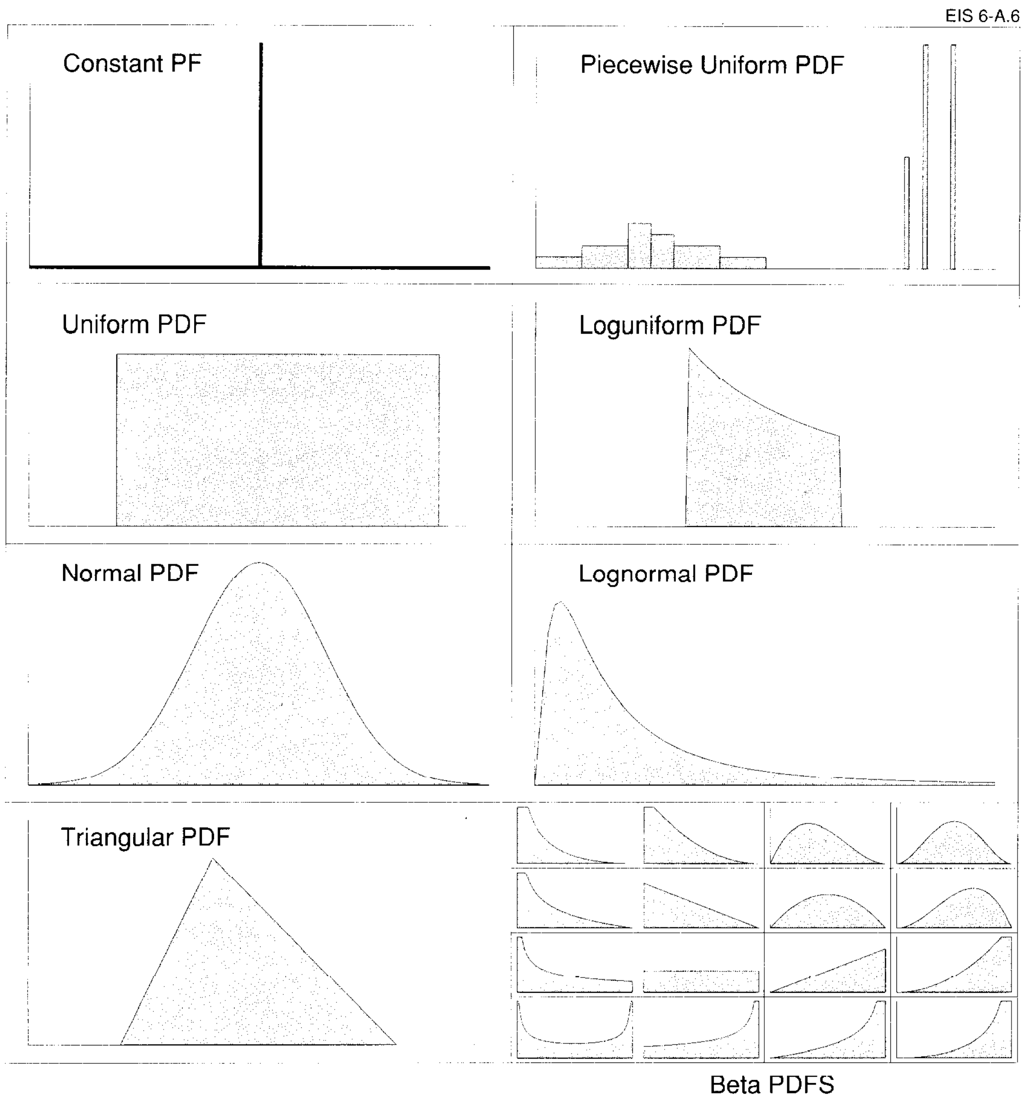

FIGURE A-6: Sample Probability Density Functions Used in SYVAC3-CC3

These plots show the different types of PDFs that are available in SYVAC3-CC3. The figure for the beta PDF illustrates the many possible shapes of this function. In addition to the distributions shown here, SYVAC3 also supports correlated normal and lognormal distributions, where the correlated parameter has values that depend statistically on an independent normal or lognormal parameter. Stephens et al. (1989, 1993) provide guidelines for selecting PDFs.

A.3.4 EXAMPLES OF THE APPLICATION OF SYVAC

As implied by their acronyms, both SYVAC3 and CC3 are the third generation of a family of related computer codes (Goodwin et al. 1987a). The development, application and use of SYVAC3-CC3 has been achieved by building on the experience obtained with two prior generations of code. We list below some studies that have influenced the use of SYVAC3-CC3 in the postclosure assessment. They are summarized in Figure A-7.

The first generation of the SYVAC family is now called SYVAC1 (Dormuth and Quick 1980, Dormuth and Sherman 1981). Its applications are documented in three assessment studies:

- The first interim assessment of the concept for disposal of Canada's nuclear fuel waste in plutonic rock (Wuschke et al. 1981). This study used a relatively simple system model and about 30 sampled parameters.

- Assessments of seabed disposal of fuel recycle waste, as part of the work performed by the Seabed Working Group of the Nuclear Energy Agency of the OECD (Wuschke et al. 1983, Guvanasen 1987).

- An assessment of the disposal of intermediate-level reactor waste, for the Environmental Authority of the Chalk River Laboratories (Guvanasen 1985).

These three studies indicated that it was practical to implement the SVA approach. The SYVAC1 code was transferred to the U.K. Department of the Environment in the early 1980s and forms the basis for versions referred to as SYVAC 'A' in their publications (Thompson et al. 1984, Thompson 1986, Hall and Thompson 1985).

Subsequent work led to the development of SYVAC2 (Sherman et al. 1987). The two main applications of SYVAC2 were

- A second interim assessment of the concept for disposal of Canada's nuclear fuel waste in plutonic rock (Wuschke et al. 1985). This study used a more detailed system model containing over 500 sampled parameters (Heinrich 1984b, Mehta 1985, LeNeveu 1986). It also examined two alternative waste matrices: used-fuel bundles and waste that could arise from the recycling of used fuel.

- An assessment similar to the second interim assessment described above, except that the emphasis was on potential chemical toxicity impacts associated with the concept for the disposal of Canada's nuclear fuel waste (Goodwin et al. 1987c).

The SYVAC3 code is the latest generation of the SYVAC family. Its most important application is described in this document. It forms the basis of the quantitative analysis for the postclosure assessment of one possible implementation of the concept for disposal of Canada's nuclear fuel waste, using SYVAC3-CC3.

GENERATION OF SYVAC	APPLICATIONS
SYVAC1	Concept for the disposal of Canada's nuclear fuel waste (Wuschke et al. 1981) Seabed disposal of fuel recycle waste (Wuschke et al. 1983; Guvanasen 1987) Geological disposal of intermediate-level reactor waste (Guvanasen 1985)
SYVAC2	Concept for disposal of Canada's nuclear fuel waste, including used fuel and fuel recycle waste (Wuschke et al. 1985) Concept for the disposal of Canada's nuclear waste, focussed on chemical toxicity impacts (Goodwin et al. 1987c)
SYVAC3	Quality assurance of the Uranium Tailings Assessment Program (Goodwin et al. 1987b) PSAC code intercomparisons (PSAC 1987; 1989; 1990; 1993) Assessment of a disposal option for low-level waste in New York State (ACRES 1989) Assessment of a near-surface engineered vault for low-level radioactive waste (Rattan 1993)

FIGURE A-7: Summary of Applications of the SYVAC Family of Computer Codes

Other applications of SYVAC3 are

- Two comparison studies carried out to provide quality assurance of the Uranium Tailings Assessment Program (UTAP) (Goodwin and Andres 1986, Goodwin et al. 1987b). The Canadian National Uranium Tailings Program developed UTAP for the long-term assessment studies of uranium mill and mine tailings (Holmes 1987, SENES 1985, 1986)

- Four international code comparisons: the Level 0, Level E, Level 1A and Level 1B exercises (PSAC 1987, 1989, 1990, 1993), organized by the PSAC User Group.

- A contract study for the Department of Environmental Conservation of New York State, to examine one of the disposal options for low-level radioactive waste (ACRES 1989).

- A preliminary safety analysis of an Intrusion Resistant Underground Structure (IRUS) for near-surface disposal of low-level waste (Rattan 1993).

These applications, each using fundamentally different system models, indicate that the SYVAC family of codes can be successfully adapted to handle a range of assessment tasks.

A.3.5 STATISTICAL CONVERGENCE OF SVA RESULTS

In this section, we provide more detail on the statistical foundation of the SVA approach. Of particular interest is the convergence of results; that is, the degree of confidence associated with the estimated mean of variables such as annual dose at 10^4 a.

Note that the "confidence" referred to here must be qualified: it refers only to a statistical measure of the results from a finite number of simulations in which the parameter values have been randomly selected from their PDFs.

Our applications of SVA and SYVAC are conducted in circumstances where substantial uncertainty affects the results. In the case of nuclear fuel waste disposal, uncertainty arises because much of the disposal system is natural, rather than engineered to specifications, and because the timescales of concern are extremely long. Much of this uncertainty is represented in the PDFs for the parameters in the CC3 model and is reflected in the distribution of impact estimates. Statistical measures of confidence apply only to this variation of the impact estimates. They do not deal with other kinds of uncertainties, such as uncertainty in the validity of the models and data.

To demonstrate the degree of statistical confidence in (or convergence of) the results, we first analyze the observed statistics of a sampled parameter whose intrinsic statistical properties are known. We then repeat the analysis for the mean ADE obtained using SYVAC3-CC3.

The sampled parameter chosen was PRECIP, which represents the annual precipitation falling at the reference disposal site in SYVAC3-CC3. This parameter is described using a normal PDF with the following attributes (Davis et al. 1993): a mean and standard deviation of 0.78 and 0.11 m/a respectively and a lower truncation limit of 0.20 m/a.

To demonstrate that SYVAC3-CC3 sampled correctly the specified PDFs, we have analyzed the values of PRECIP used in the simulations. Table A-1 summarizes some statistics from 10 000 randomly selected samples:

TABLE A-1

STATISTICS FOR THE PARAMETER PRECIP

Statistic	Actual Value*	Estimated Value*
Mean	0.78	0.7812
Standard deviation	0.11	0.1110
Standard error	0.0011	0.0011
Lower 95% confidence bound**	--	0.7790
Upper 95% confidence bound**	--	0.7834

* The "actual" values are those used to define the probability density function (PDF) for PRECIP, a sampled parameter in SYVAC3-CC3 that represents total annual precipitation. The "estimated" values are the statistics calculated from 10 000 simulations, in which values for PRECIP were randomly selected from its PDF. The dimensions of all values are m/a.

** Confidence bounds apply to the estimated mean value and are calculated using Student's t-distribution with 9999 degrees of freedom.

- The mean and standard deviation of the sampled values should approximate closely the mean and standard deviation of the normal distribution from which they were sampled. The first two rows of the table show excellent agreement between the actual and estimated statistics.

- The standard error, representing the statistical variability of the sample mean, is the standard deviation divided by the square root of N, where N is the number of simulations (10 000 in this case). The standard deviations agreed exactly.

- The lower and upper 95% confidence bounds define a range that would contain the theoretical mean of PRECIP (0.78 m/a), 19 times out of 20. They are 1.96 standard errors below and above the sample mean.

Part (a) of Figure A-8 provides a visual comparison. It shows a histogram of the 40 000 randomly sampled values for PRECIP and the theoretical curve of the normal PDF whose attributes are the same as the attributes for PRECIP. From a visual inspection, the PDF and the histogram agree quite well.

Parts (b) and (c) of Figure A-8 give more quantitative evidence that PRECIP was sampled from a normal PDF. These two plots are cumulative normal probability plots, with sample values along the horizontal axis and cumulative percents along the vertical axis. The probit scale of the vertical axis is

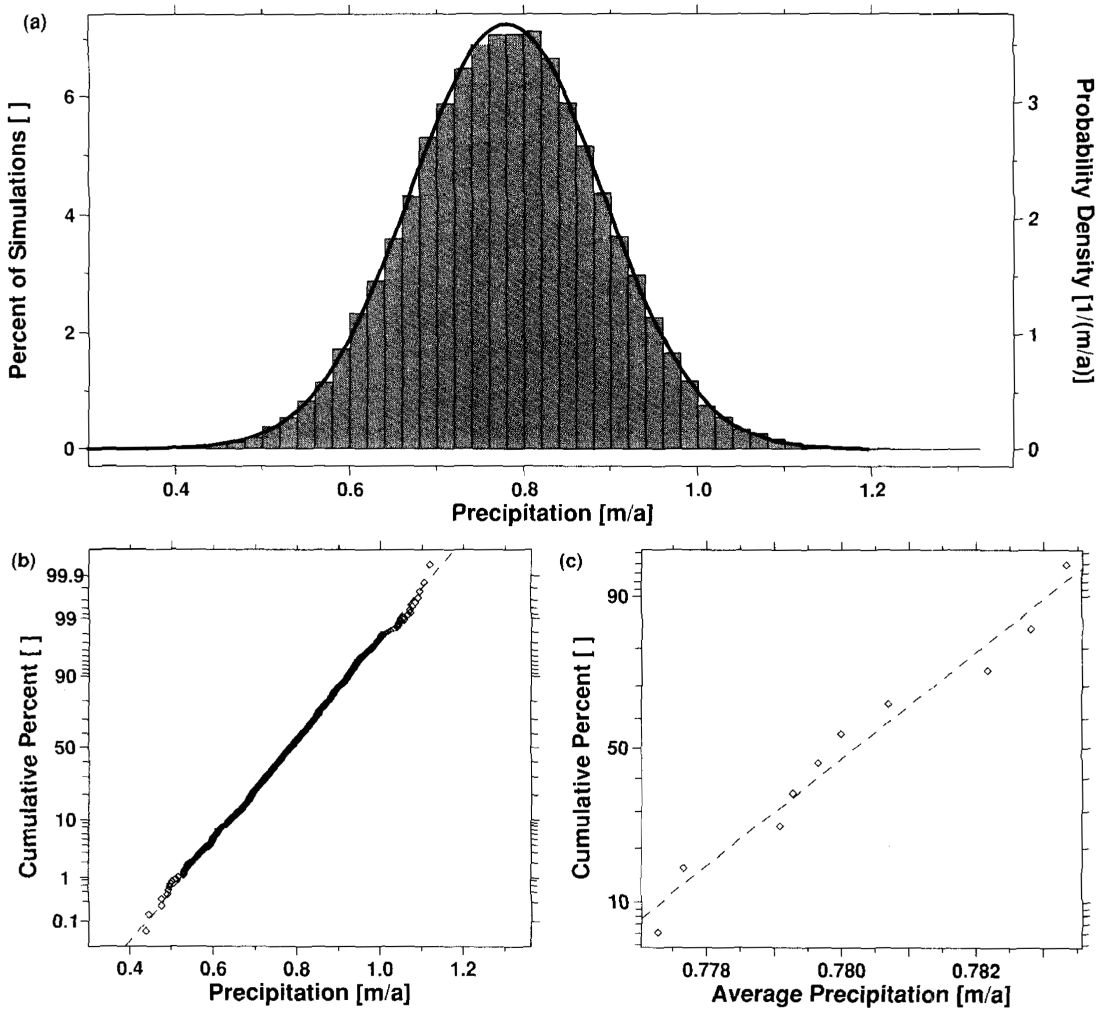

FIGURE A-8: Distribution of the Variable PRECIP from Simulations Using SYVAC3-CC3

PRECIP is a parameter used to represent the annual precipitation falling on the disposal site. Its values are sampled in SYVAC3-CC3 from a normal probability density function (PDF) with a mean, standard deviation and lower limit of 0.78, 0.11 and 0.2 m/a respectively.

Part (a) of the figure is a composite plot. The solid line is the theoretical PDF for PRECIP. The histogram shows the frequencies of different values that were observed in 40 000 random samples. As expected (and as required), the PDF and histogram match closely. (The units of the vertical axis follow from the requirement that the integrated probability must equal unity.)

Parts (b) and (c) are cumulative normal probability plots. The vertical axis is the cumulative percentage of values of PRECIP that are less than or equal to the corresponding values on the horizontal axis. The probit scale on the vertical axis was chosen such that the points would fall on a straight line if the values of PRECIP were sampled from a normal distribution. Part (b) uses 40 000 randomly sampled values of PRECIP, and the linear relationship (R^2 = 0.999) strongly suggests that the data were sampled from a normal distribution. Part (c) uses 10 values, each being averages of 4000 simulations. The fit in (c) is poorer (R^2 = 0.983) than (b) because it contains a smaller number of points. However, the procedure used to develop part (c) can be used to estimate confidence bounds even when the original data are not normally distributed.

These results suggest that the sampled values of PRECIP have been selected from a normal PDF and, therefore, provide confidence that SYVAC3-CC3 has correctly sampled parameter values.

such that a straight line would result if the values were sampled from a normal distribution.

- Part (b) shows 40 000 randomly sampled values of PRECIP. The regression line drawn through the points in the plot is statistically an excellent fit and, therefore, indicates that the distribution of PRECIP is close to a normal PDF.

- Part (c) uses 10 average values of PRECIP; each average is calculated from an independent set of 4000 randomly selected simulations. The points in the plot also fit reasonably well to a straight line, although the fit is worse than in part (b) because of the smaller number of points.

This type of plot is important in our analysis of convergence. Suppose, for example, that another parameter, PARAM, was sampled from another type of PDF (not a normal PDF). The central-limit theorem (Sokal and Rohlf 1981) guarantees that average values of PARAM would be nearly normally distributed, providing that the averages are calculated from a set of independent groups of values and that each group contains a sufficiently large number of sampled values. We can then use this fact to derive confidence bounds for PARAM, by treating the average values as samples of a normal distribution.

We can now apply this analysis to mean annual dose. Compared with the analysis for PRECIP, two extra properties must be taken into consideration for mean annual dose:

- The actual distribution of annual doses is unknown and, therefore, we do not have an available value to check for convergence; and

- Estimated annual doses are a function of time and, therefore, the frequency distribution of annual doses may display a different pattern at different simulation times. Thus the analysis of convergence must be repeated at several representative points in time over the period of the simulations.

Figure A-9 was produced in the same way as Figure A-8, except that it deals with mean annual dose at 10^4 a. Part (a) of the figure is a frequency distribution of annual doses obtained from 40 000 simulations. The distribution is strongly skewed to small values, and the mean annual dose is dominated by a few simulations with relatively large ADEs. Part (b) is a cumulative normal probability plot involving individual simulations. Clearly the points are a poor statistical fit to a straight line, especially for large values of annual dose. Therefore, the data are unlike normally distributed data, and standard confidence limits do not apply.

However, we can use part (c) of Figure A-9 to estimate confidence limits. As noted earlier, the central-limit theorem states that the average values of annual dose will tend to be normally distributed, even though annual dose itself is not. Part (c) demonstrates that averages of annual dose using 4000 simulations are large enough to have a mean annual dose at 10^4 a

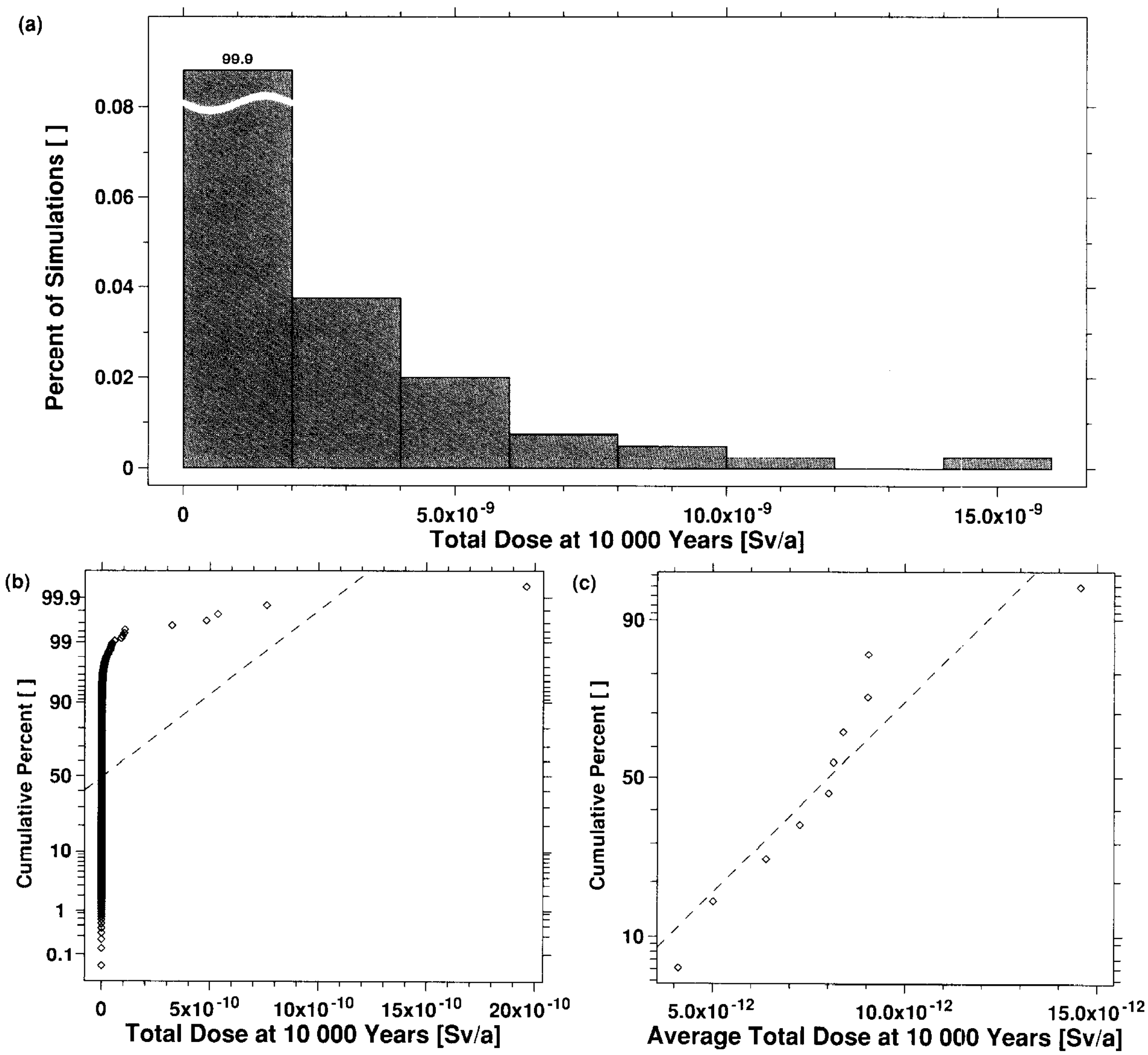

FIGURE A-9: Distribution of Annual Doses at 10^4 a from Simulations Using SYVAC3-CC3

Part (a) is a histogram showing the frequencies of occurrence of annual dose at 10^4 a from 40 000 simulations. Note that the first bar of the histogram has been cut off so that the other bars could be shown. The distribution is strongly skewed to the left (see also Figure 6-17 in Section 6.5.2 in the main text).

Parts (b) and (c) are cumulative normal probability plots (compare with Figure A-8, parts (b) and (c)). Part (b) uses values of mean annual dose from 40 000 randomly sampled simulations. The poor linear relationship (R^2 = 0.206) confirms that the data are not normally distributed. Part (c) uses 10 averages of annual dose, each being averages of 4000 simulations, and shows a better linear relationship (R^2 = 0.931), as predicted by the central-limit theorem. Because the data in part (c) are approximately normally distributed, they can be used to estimate confidence bounds.

that is approximately normally distributed. (The choice of 4000 simulations used in the figures was arbitrary. Similar results would be obtained with eight groups of 5000 simulations. With more groups and fewer simulations in each, the fit tends to get worse.) We can then use standard confidence limits for the 10 average data points in part (c) and estimate confidence bounds for mean annual dose at 10^4 a.

Similarly, we can repeat the analysis for mean annual dose at other times, as is shown in Figure A-10. Part (a) of this figure shows the distribution of annual dose at 10^5 a. Although the annual doses are greater, they are less skewed than at 10^4 a. The plot of single simulations, shown in part (b), confirms that the annual doses at 10^5 a are not normally distributed. However, the fit of the ten average annual doses to a straight line in part (c) of the figure suggests that the average annual doses are normally distributed.

The corresponding statistics for annual dose at 10^4 and 10^5 a are summarized in Table A-2. The standard deviation quoted is calculated from the ten annual doses obtained by averaging ten sets of 1000 simulations (from the first 10 000 simulations discussed in Figures A-9 and A-10). Note that the standard error is about one third of the standard deviation because there are only N = 10 observations that can be considered to be normally distributed (in the analysis of PRECIP, the ratio was about 1/100 because there were 10 000 observations considered to be normally distributed). The 95% confidence bounds are 2.26 standard errors below and above the sample mean. The value 2.26 comes from a t-distribution with 9 degrees of freedom. It differs from the value 1.96 in the PRECIP example, because PRECIP has 9999 degrees of freedom (Sokal and Rohlf 1981).

Table A-2 also includes for comparison the lower and upper 95% Chebyshev confidence bounds. Chebyshev bounds on mean dose at the 95% confidence level are 4.47 standard errors from the mean (PSAC 1989). The Chebyshev bounds are valid for any distribution whatever, provided that the estimated standard error is approximately correct. However, we believe that the 95% confidence bounds, as estimated above, more accurately represent the bounds for mean annual dose that were calculated using SYVAC3-CC3.

A.4 SENSITIVITY ANALYSIS

A.4.1 INTRODUCTION

Simulations of the performance of a waste disposal facility reveal possible environmental impacts. Sensitivity analysis allows us to extend our understanding of the processes involved, by examining questions such as the following ones.

- How sensitive are the estimates of impact to changes in the modelling of the processes?

- If individual parts of the system model are changed, which have more significant effects on the estimates of impact?

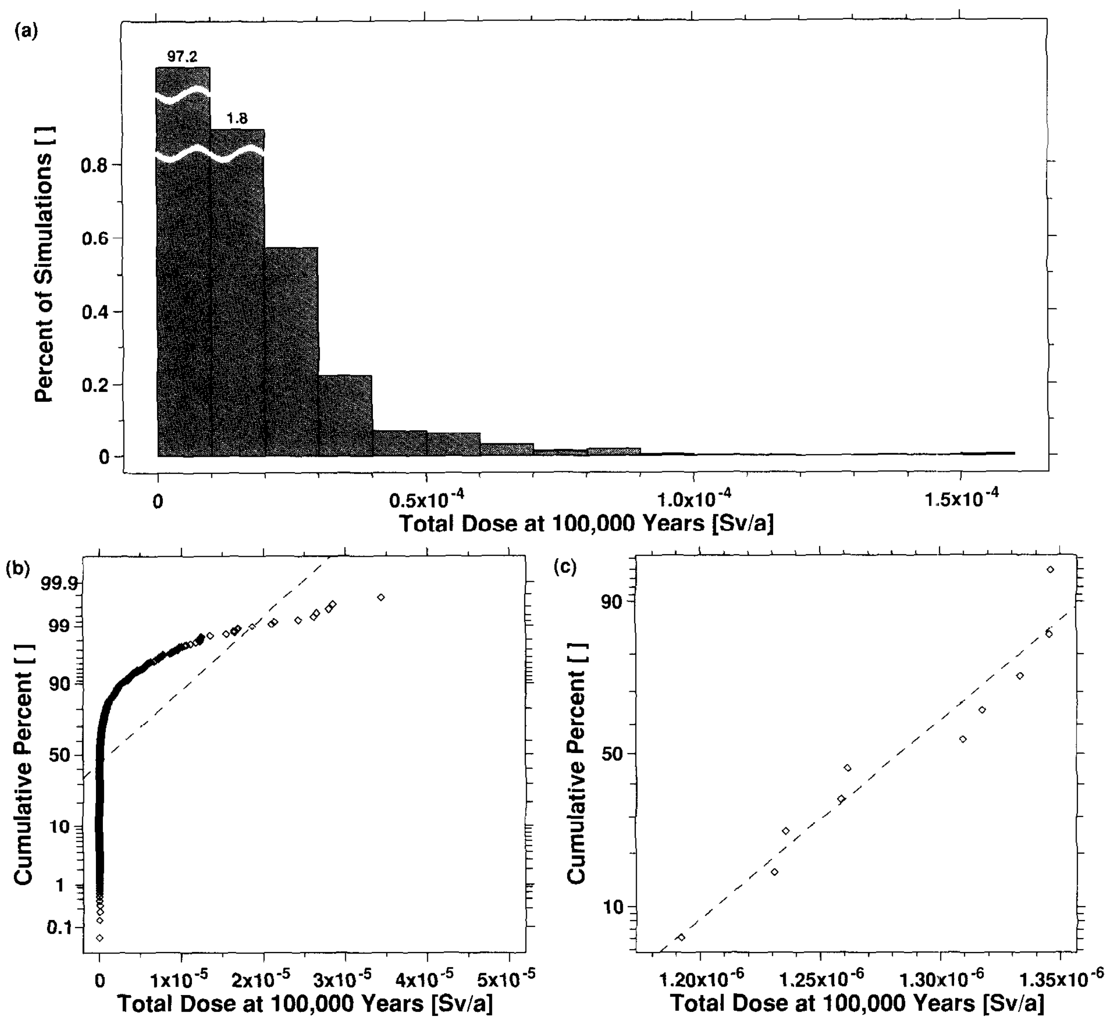

FIGURE A-10: Distribution of Annual Doses at 10^5 a from Simulations Using SYVAC3-CC3

Comments are as for the previous figure, except that the data are at 10^5 a. The distribution is strongly skewed but not as much as in part (a) of Figure A-9. The straight line in part (c) shows a good linear relationship (R^2 = 0.967), indicating that the results can be used to estimate confidence bounds.

TABLE A-2

STATISTICS FOR MEAN ANNUAL DOSE

Statistic*	Mean Annual Dose (Sv/a) at 10^4 a	10^5 a
Mean	7.6×10^{-12}	1.3×10^{-6}
Standard deviation of 10 estimates of the mean, each from 1000 simulations	5.8×10^{-12}	1.2×10^{-7}
Standard error	1.8×10^{-12}	3.8×10^{-8}
Lower 95% confidence bound**	3.5×10^{-12}	1.2×10^{-6}
Upper 95% confidence bound**	12.0×10^{-12}	1.4×10^{-6}
Lower 95% Chebyshev confidence bound	0.0	1.1×10^{-6}
Upper 95% Chebyshev confidence bound	1.6×10^{-11}	1.5×10^{-6}

* The statistics were calculated from the results of SYVAC3-CC3 for 10 000 randomly selected simulations (the first 10 000 simulations described in Chapter 6 in the main text). Because the ADEs are a function of time, the statistics for the mean annual dose are also a function of time. The statistics given in the two columns are for the mean annual dose at 10^4 and 10^5 a.

** Based on Student's t-distribution with 9 degrees of freedom.

- Are there any design or siting changes that would lead to significant changes in the estimated performance?

- How can we reduce the magnitude <u>and</u> uncertainty associated with the estimated impacts?

The general procedure involved in sensitivity analysis is simple: change some aspect of the system model and data and observe any difference in the estimated performance. If the difference is significant, the change is important. For example, suppose the assessment simulations are re-done without one of the radionuclides. If ADEs are reduced by a significant amount, then the presence of that radionuclide in the simulation is important. If ADEs do not change significantly, then that radionuclide does not contribute much to environmental impacts.

The foremost objective of sensitivity analysis is to identify important features of the system. Then analysts search for the underlying reasons for the observed behaviour of the important features to confirm their understanding of the system. In addition to a general quest for understanding, an assessment analyst may have other specific objectives. Sensitivity analysis may contribute to activities such as

- *Development of derived constraints.* Derived constraints are applied to the design or siting of a disposal system to improve the estimated performance. One effective design constraint adopted for the disposal system analyzed in this study relates to the location of the vault with respect to fracture zone LD1 (Section 6.2 in the main text).

- *Setting of research priorities.* If the estimated performance of a disposal system is found to depend mainly on our understanding of a single process or feature, such as chemical retardation, further laboratory or field research may be warranted to develop more accurate models and parameter distributions for this process. Research priorities can be directed toward reducing estimated impacts (such as mean annual dose) or toward reducing the uncertainty in estimated impacts (such as the variability in mean annual dose). Section E.7 of Appendix E describes such a study.

- *Testing of models and data.* Many different procedures are used to check the models and data, and results from sensitivity analyses play an important role. In our experience, fractional factorial analysis (described below) is especially effective because it uses many combinations of near-extreme parameter values. These unlikely combinations stress the models and their computer implementations and help to identify possible flaws. Computer models can, therefore, be rendered more robust and reliable by subjecting them to sensitivity analysis of this type. Many of the results described in Sections D.5 to D.8 of Appendix D have contributed to the testing of SYVAC3-CC3.

- *Development of better models and data.* Often it is most practical to develop a preliminary model of some process, with assumptions made such that the impacts are overestimated. Sensitivity analysis can then be used to examine the preliminary model to determine the magnitude of estimated impacts. If impacts can be significant, then refinements to the preliminary model might be indicated, to produce a more accurate model. Sensitivity analysis can also be valuable in refining the data used by the models.

- *Development of a clarified description of the disposal system.* In a description of a disposal concept, as in this volume, it is important to identify the main features that control system behaviour. For instance, the total ADE up to 10^5 a is due to only ^{129}I and ^{14}C, with little contribution from all other radionuclides. Sensitivity analysis helps to focus on these key characteristics of the system.

A.4.2 IDENTIFYING IMPORTANT FEATURES

An important feature is one which, when changed, leads to significant changes in system behaviour. Changes to a feature can be modification, removal or addition of the feature:

- *Modifications.* The most common changes made for sensitivity analysis are modifications, especially to parameter values or distributions. To a great extent the features and processes in an assessment model are represented by sets of parameters. Such features and processes can then be readily modified by changing the values of appropriate parameters.

For example, SYVAC3-CC3 has parameters that determine whether or not a well is used, whether lake sediment is used as soil, and whether irrigation is employed. Other continuous parameters, such as diffusion and retardation factors, control the extent to which processes such as diffusion and sorption affect the results of the simulation. Because most changes of interest can be made by modifying parameter values or distributions, sensitivity analysis of SYVAC3-CC3 usually involves changing one or more parameters and observing any changes in the simulation results.

- *Removals.* Omitting a nuclide in a simulation is an example of a removal change. Similarly, one could remove an exposure pathway in the biosphere model, such as the irrigation of the garden; a feature, such as the well in the geosphere model; or constraints, such as solubility limits in the vault model.

  In SYVAC3-CC3, omitting a nuclide is a simple change to the corresponding input file for the system model. Removing other features is often a matter of changing one or more parameter values in the input file to an extreme value, such as increasing all solubility limits to a large value that effectively removes the effects of precipitation of nuclides.

- *Additions.* These are rare in sensitivity analysis. Adding a new feature such as a fracture or an additional type of waste, or a new process such as colloidal transport, will typically require model changes and not modification of existing parameter values. Additions usually require large investments in time and effort and, if made, are subsequently retained as a permanent feature of the model.

  Additions for sensitivity analysis in SYVAC3-CC3 are most likely to occur in components of the model that are controlled by tables of data, rather than code. For instance, a new nuclide can be added to the assessment by making data changes only. Another example is the geosphere network model, where the locations of "nodes" and "segments" are controlled by a data file. A new feature of the network may be added by introducing new nodes and segments with a data change.

The changes made for sensitivity analysis can be classified in other ways, such as whether the analysis is deterministic or probabilistic:

- *Deterministic sensitivity analysis:* Modify the value of a parameter. As suggested in part (a) of Figure A-11, the outcome is a difference in the *value* of a consequence variable. This "classical" sensitivity analysis is probably the most common approach used to study a model.

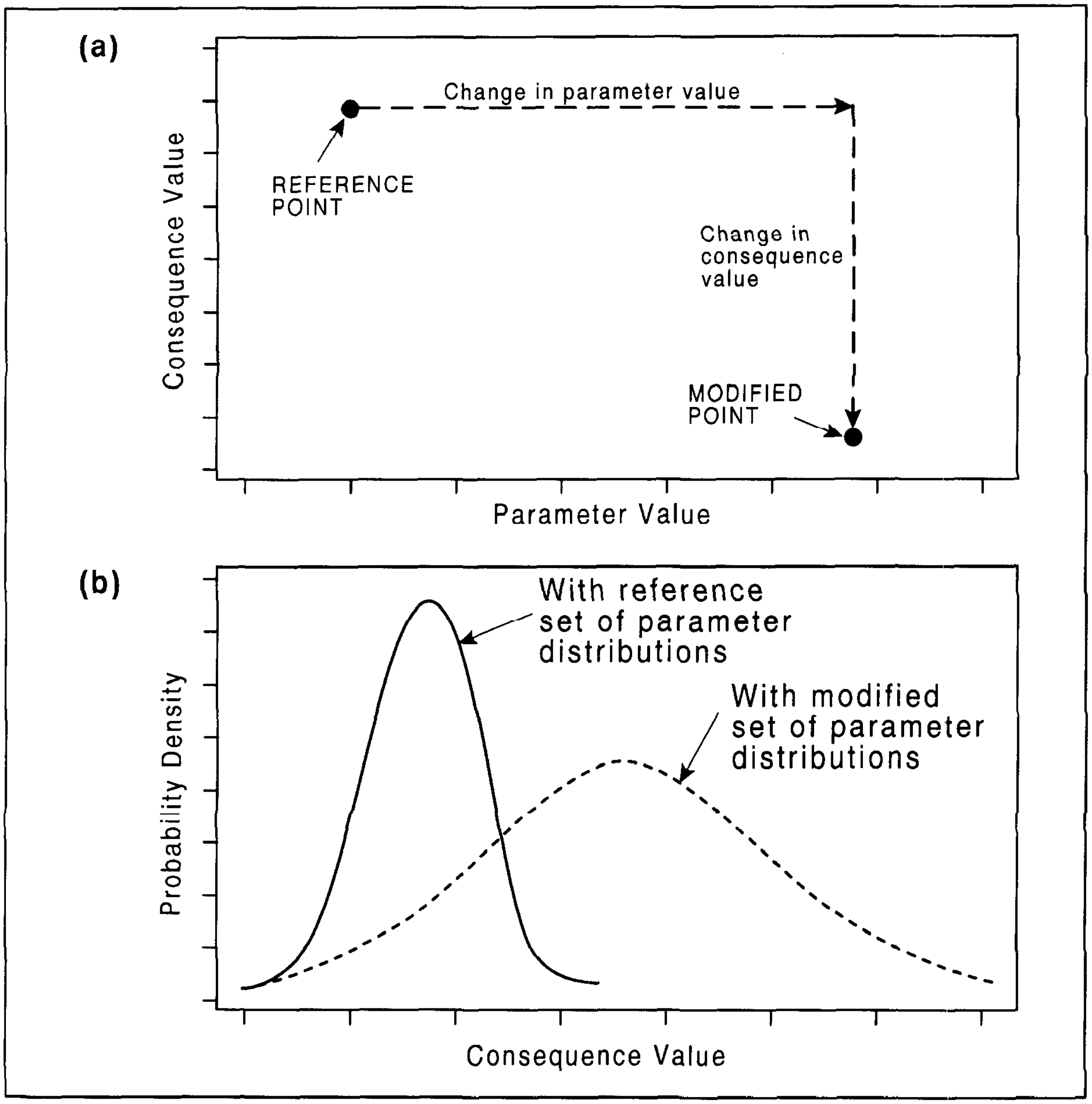

FIGURE A-11: Comparison of Deterministic and Probabilistic Sensitivity Analysis

In deterministic sensitivity analysis, a parameter is changed from a reference value to a modified value. As a result, the consequence variable also changes in value. This effect is illustrated in part (a): the reference point corresponds to the original parameter and consequence values, and the modified point corresponds to the changed parameter and consequence values. In probabilistic sensitivity analysis, a parameter distribution is changed. The distribution of a consequence variable changes as a result, as illustrated in part (b). Note that both types of sensitivity analysis may involve more than one parameter and more than one consequence.

In applying deterministic sensitivity analysis to SYVAC3-CC3, we usually restricted the modified values to small variations about the median value (although full-range studies were also made). The corresponding results then apply to the situation where all parameters take on values near their median value. The results are equivalent to partial derivatives of an output variable with respect to a single parameter.

- *Probabilistic sensitivity analysis:* Modify the PDF of a parameter, or select values that span the entire range of possible values of a parameter. Part (b) of Figure A-11 suggests that the outcome of a modified PDF is a difference in the *distribution* of a consequence variable, implying a possible difference in its mean consequence value and its variability. Using selected values from the parameter's range will have a similar effect. (Probabilistic sensitivity analysis is related to uncertainty analysis because both deal with the propagation of uncertainty from parameters to consequences. Probabilistic sensitivity analysis, however, provides more information because it includes the probability of different occurrences of the values of a parameter in its PDFs, and the method typically examines a suite of these values. By contrast, uncertainty analysis will typically assume a uniform PDF for all parameters and examine only extreme values.)

  In applying probabilistic sensitivity analysis to SYVAC3-CC3, we most frequently used values selected from the high and low extremes of the parameter PDF, as well as the median value, to identify important parameters. A systematic method, described below, was used simultaneously for all parameters, and the corresponding results take into account the entire range of uncertainty of all parameters. The results are also approximately equivalent to evaluating the average effect (and not a partial derivative) of changing one parameter when all other parameters are simultaneously free to vary across their entire range of possible values.

Parameter changes made for sensitivity analysis can be further classified as either feasible or exceptional:

- *Feasible changes:* For a parameter, choose values that lie within a defined range. For instance, in some studies using the SYVAC3-CC3 model, we vary the number of people in the critical group from one to 36, the range specified for the reference disposal system (Davis et al. 1993).

- *Exceptional changes:* For a parameter, choose values that lie outside its normally defined range. Continuing from our example above, using a critical group with 100 people would be an extraordinary change because the specified upper limit (for the probabilistic assessment) is 36. Exceptional changes are usually made to investigate different design specifications. We might use an unusually large critical group to examine the effect of large well water demand. Another example is given by the thickness of the buffer; it is fixed at 0.25 m in the reference disposal system. An exceptional change would be to set the thickness to 1.0 m. Sections 6.2 and 6.6 in the main text document some examples, including the use of a thicker buffer to investigate the effects of an alternate design that would increase the amount of buffer surrounding a container.

When sensitivity analysis is carried out using parameter changes, it can reveal the parameters that have an important effect on consequences. The *importance* of the parameter can often be established using abstract statistical tests. Further work by the analysts then focuses on determining *why* it is important. This last element of sensitivity analysis often requires a detailed understanding of the system model. It can also draw on the results of the thousands of randomly sampled simulations to illustrate what the effects are.

For example, sensitivity analysis of results from SYVAC3-CC3 has identified the importance of a variable called VSCALE. This parameter describes the groundwater velocity in the rock of the geosphere, with large values of VSCALE corresponding to higher groundwater velocities. Its effects are complex. For some simulations, a large value of VSCALE leads to significantly increased ADEs, whereas in other simulations a small value of VSCALE leads to significantly increased ADEs. Given this information, a further examination of the results shows that these differential effects are (in part) related to the different rates of radioactive decay of different contaminants (Section D.7 of Appendix D provides more details):

- For a nuclide such as ^{14}C, with a relatively short half-life of 5730 a, faster groundwater transport brings more of the nuclide to the biosphere before it decays. Hence larger values of VSCALE could lead to increased ADEs from ^{14}C.

- For a nuclide such as ^{129}I, with a much longer half-life of 1.6×10^7 a, radioactive decay has a small effect during the time required for groundwater transport. However, because slower groundwater transport reduces the amount of dispersion and mixing, it follows that smaller values of VSCALE could lead to increased ADEs from ^{129}I.

A.4.3 METHODS USED IN THE POSTCLOSURE ASSESSMENT

Sensitivity analysis of a SYVAC3 model is typically done in a three-stage process:

1. Screening analysis using feasible changes in parameter values identifies important parameters. Expert knowledge and systematic experimentation using statistical designs (described below) both contribute to the screening process. The result is a list of parameters that require further investigation because they have a strong influence on the behaviour of the model.

2. Detailed sensitivity analysis is applied to each important feasible change. The important parameters are varied systematically within their ranges to determine the nature of and the reasons

for the observed cause-effect relationships, or a large set of randomly sampled simulations are statistically evaluated with the same goal.

3. Exceptional analysis is used to explore specific situations or possible derived criteria for the disposal system. Parameters are given values outside their normal ranges to generate the information required to understand special cause-effect relationships.

We have found that these last two steps are relatively straightforward; that is, once a parameter has been identified as important, the reasons for its importance are usually easy to decipher.

In contrast, the first step of parameter identification is usually the most difficult. This is especially true for models containing a large number of parameters, as is the case for SYVAC3-CC3. Thus we use the remainder of this section to elaborate on the use of screening analysis to identify important parameters.

Screening analysis can use information from any source to identify important and feasible changes in simulations. For example, a model developer might target a particular parameter that he suspects of being important. Or analysts may know from simulations with earlier models that a particular nuclide or pathway is likely to be important. These pieces of information are significant contributions, although they may not always be systematic and comprehensive.

There are a number of more structured methods that could be used to identify important parameters. Two computer codes that have been applied to the analysis of SYVAC2 results are ANSENS, an acronym for ANalyze SENSitivity, (Frech and Andres 1987) and CANAL, an acronym for Correlation ANALysis (Walker 1986). Other methods are described by Saltelli and Marivoet (1990) and Saltelli and Homma (1992) and Saltelli et al. (1993).

Having examined many of these methods, we concluded that another approach is better suited for use with SYVAC3-CC3. This approach, discussed in the following section (see also Saltelli et al. (1993) and Andres and Hajas (1993)), is based on a statistical experimental design. It is used extensively to identify important parameters. Another method, conventional linear regression analysis, is used to compare and confirm the results of the statistical design.

A.4.3.1 Statistical Experimental Designs

Our experience and studies have revealed one method that is well suited to the analysis of SYVAC3-CC3. Most of our screening analysis results have come from carrying out simulations according to a "statistical experimental design"; that is, experiments are planned in such a way that appropriate data will be collected (Montgomery 1984). These data may then be analyzed by statistical methods. In our postclosure assessment studies

- an experiment is equivalent to a single computer simulation using SYVAC3-CC3,

- a statistical experimental design is a set of such simulations, in which the value of every parameter is predetermined,
- planning the experiments means selecting a set of particular values for all the sampled parameters used by the model in the set of simulations, and
- the set of parameter values and corresponding estimated consequences are then evaluated using a suitable statistical analysis to identify the important parameters.

The selection of parameter values for SYVAC3-CC3 is carried out with the aid of the computer code SAMPLE (Andres 1987). The SAMPLE code can generate a set of parameter values for several types of statistical designs. The most commonly used type is the fractional factorial design, which is a subset of a full factorial design.

In a full factorial design, there are experiments covering all possible combinations of permitted parameter values. The word "permitted" in this statement is needed because most parameters can take on an infinite number of possible values, and it is customary with factorial designs to restrict such parameters to a few discrete values. In a 2^n factorial design, there are n factors, each restricted to just two values: usually a small value and a large value.

With two values and two parameters, four experiments are required. With two values and twenty parameters, over one million experiments are needed. As noted in Section A.3.3, SYVAC3-CC3 requires about 4000 parameters for simulations containing ten contaminants; a full factorial design would require an unacceptably large number (2^{4000}) of experiments. Therefore, we investigated an abbreviated version, the "fractional" factorial design. This design uses fewer simulations, chosen to achieve the maximum information about parameter sensitivity.

An effective fractional factorial design can be much smaller than the corresponding full factorial design. Resolution IV fractional factorial designs (Montgomery 1984) are particularly attractive. In such a design, the effects of each parameter can be separated from the effects of other parameters and also from the nonlinear interaction effects of any two parameters. The size of such a design for n parameters is at least 2n; thus for 4000 parameters, at least 8000 simulations are required.

For the sensitivity analysis of SYVAC3-CC3, we applied our previous experience to develop a variation on the usual fractional factorial designs. Our studies of the CC3 and related system models show that a handful of parameters usually controls the behaviour of the model. For example, the results in Chapter 6 in the main text indicate that ^{129}I and ^{14}C are the only significant contributors to the ADE. Thus several hundreds of parameters, used to describe the behaviour of other radionuclides, cannot be important.

For this situation, we have developed a method, iterated fractional factorial design (IFFD), that typically requires only a few hundred simulations to screen 4000 parameters.

To explain IFFD, we first assume that there is only one important parameter in the system model, and that this parameter leads to large results when it takes on large values and to small results when it is small.

Consider the simple case where there are just eight parameters in the system model. Figure A-12 illustrates an IFFD for a two-value analysis. It uses one possible combination of 16 simulations that satisfies the requirements:

- Each of the eight parameters has an equal number of simulations with high (H) and low (L) values.

- For any pair of parameters, there are equal numbers of simulations where both parameters are high and both are low or where one is high and the other is low (the figure shows an equal number of H-H, H-L, L-H and L-L combinations).

- For any three parameters, there are equal numbers of simulations involving each combination of high values and low values (the figure shows equal numbers of combinations such as H-H-H, H-H-L, H-L-H, and so on).

The last column in the figure shows the hypothetical results of the simulations; from an analysis of the pattern we can easily identify the single important parameter in the set of eight parameters. In practice, an important parameter is identified by a large difference in the average consequence as the parameter value changes from low to high. This difference in averages is labelled the main effect.

Figure A-13 illustrates the extension of IFFD to cases where a single important parameter is one of a set of 8, 16 and 512 parameters:

- *8 parameters.* This situation is illustrated in part (a) of Figure A-13, where the one important parameter is represented by a filled box. As discussed for Figure A-12, only 2 x 8 = 16 simulations are needed to identify the single important parameter by its main effect.

- *64 parameters.* It is possible to construct a statistical design that will identify the single important parameter using 2 x 64 = 128 simulations. But part (b) of Figure A-13 shows how IFFD can be used to identify the important parameter using only 32 simulations:

    1. The 64 parameters are arranged in a square array. The parameters can be partitioned into eight groups either by row or by column. First, all the parameters in each <u>row</u> are grouped together, and each group is treated as a single parameter. If the group is assigned a high value, then every parameter in the group must take a high value. If the group is assigned a low value, then every parameter in the group must take a low value. Then in 16 simulations, it will be possible to identify the one group out of eight containing the important parameter (that is, the parameter having the largest main effect). At this stage, there is no way of determining which parameter in the group is causing the effect.

Simulation Number	Parameter								Result
	P1	P2	P3	P4	P5	P6	P7	P8	
1	H	H	H	H	H	H	H	H	H
2	H	L	H	L	H	L	H	L	H
3	H	H	L	L	H	H	L	L	L
4	H	L	L	H	H	L	L	H	L
5	H	H	H	H	L	L	L	L	H
6	H	L	H	L	L	H	L	H	H
7	H	H	L	L	L	L	H	H	L
8	H	L	L	H	L	H	H	L	L
9	L	L	L	L	L	L	L	L	L
10	L	H	L	H	L	H	L	H	L
11	L	L	H	H	L	L	H	H	H
12	L	H	H	L	L	H	H	L	H
13	L	L	L	L	H	H	H	H	L
14	L	H	L	H	H	L	H	L	L
15	L	L	H	H	H	H	L	L	H
16	L	H	H	L	H	L	L	H	H

FIGURE A-12: Illustration of an Iterated Fractional Factorial Design

In this example, we assume that the system contains eight parameters, P1 to P8, but only one is important. Each row represents a simulation; it uses the values for the eight parameters that appear in the first eight columns. For example, simulation 12 has low (L) values for parameters 1, 4, 5 and 8, and high (H) values for 2, 3, 6 and 7. The last column shows the "result" of the simulation (we have assumed that the result is high only when the value of the important parameter is high). From an analysis of these results, together with the parameter values, it should be clear that there is more than enough information to deduce that the single important parameter is P3. For example, simulations 1 and 9 confirm that the unknown important parameter must have a high value to give high results; from simulations 1 and 2, we deduce that the unknown important parameter is not P2, P4, P6 or P8, and so forth. The actual procedure compares, for each parameter, the average result when that parameter is high and the average when it is low. In this example, only P3 has a significant difference between its two averages, and it is clearly the single important parameter.

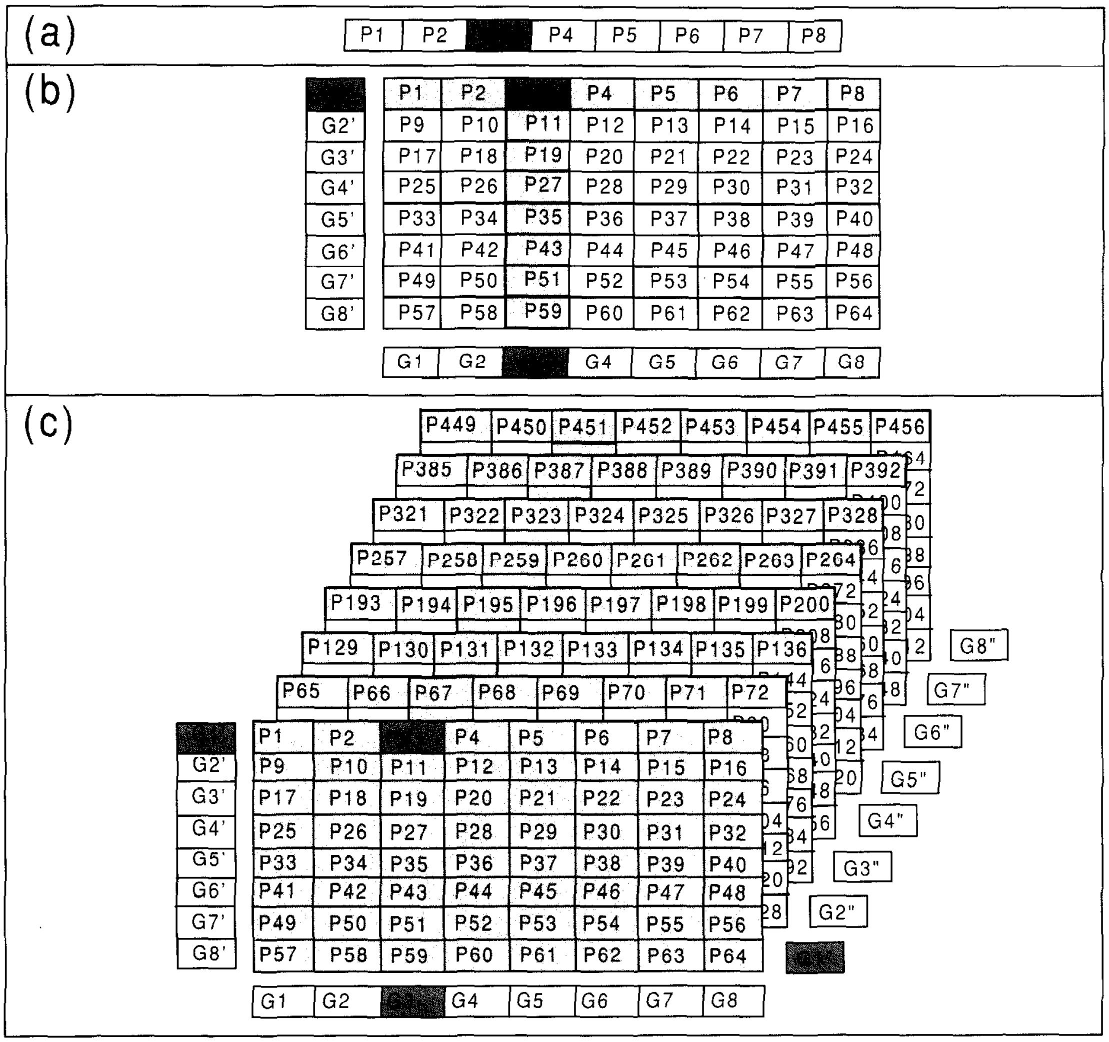

FIGURE A-13: Identification of the Sole Important Parameter from Sets Containing Many Parameters

In (a), there are only 8 parameters, and the important parameter can be identified using iterated fractional factorial analysis and 16 simulations (see Figure A-12). In (b), there are 64 parameters. They are grouped together, as shown; for example, the parameters in group G1 (column G1) include parameters P1, P9, P17, etc., and all eight parameters are sampled in the same way during the analysis of the column groups. As noted earlier, the important column group can be identified using iterated fraction factorial analysis and just 16 simulations. Similarly, the important row group can be identified with just 16 simulations. By combining the row and column analyses, we identify the important parameter using a total of 32 simulations. In (c), there are 512 parameters. These can be analyzed in 8 groups, by row, column or layer. Combining all three identifies the important parameter using a total of 48 simulations.

2. Next all the parameters in each column are grouped together, and each group is treated as a single parameter. Again, the important group can be identified with 16 simulations. But this time, because both the row and the column of the single important parameter are known, it can be uniquely identified.

- *512 parameters.* Part (c) of Figure A-13 suggests how IFFD can isolate a single important parameter out of 512 using only 48 simulations. The procedure used above is followed, except that parameters are grouped by row, by column, and by layer, and there are eight groups of 64 parameters each time. There is only one parameter that belongs to the important row, column, and level.

- *8^n parameters.* A logical extension of this approach allows us to find one important parameter out of 8^n parameters in only 16n simulations. In particular, because SYVAC3-CC3 contains about 4000 parameters and because 4096 = 8^4, in principle only 64 simulations would be needed to identify one important parameter in the SYVAC3-CC3 model. In practice, certain refinements are required, as described below.

The IFFD required the following additional innovations so that it could be implemented with SYVAC3-CC3:

- *Multiple important parameters.* The previous discussion focussed on a case with a single important parameter. In practice, there are usually several parameters that are clearly most important, and their effects can easily mask each other. To get definitive results, it has been necessary to run more groups and simulations than the 64 discussed above. Typically, 256 simulations are used with the CC3 model. Whereas 64 simulations were treated as four experiments with each having 16 simulations, 256 simulations are treated as 16 experiments with each having 16 simulations. Only the top half dozen parameters can be reliably identified in this way.

- *Random selection of groups.* When setting up groups of parameters, a systematic approach can be used, as was the case in Figure A-13. However, for the SYVAC3-CC3 analysis, groupings were made randomly. Random selection made it easier to replicate the sensitivity analysis with different groupings and to test whether important parameters were being identified consistently.

- *Three-level designs.* The discussion above is for a two-level design; that is, each parameter takes on one of two values (high or low) in each simulation. Designs with this characteristic are sufficient for models where consequence variables depend linearly on parameter values. In the SYVAC3-CC3 model, nonlinear dependencies are common; for example, in the discussion in Section A.4.2 we noted that both low and high values of the parameter VSCALE could lead to increased ADEs. It was necessary to use at least three levels to identify parameters with nonlinear effects. In each grouping, some parameters were set to a middle level in all the simulations. When this adjustment was made with care, so that it affected only a small fraction of the groupings for each parameter, it was found to give consistent three-level results. That is, another three-level design with different parameter groupings would identify the same set of important parameters.

- *Multiple consequences.* The analysis described above can be applied to different types of results. Sensitivity analysis of SYVAC3-CC3 has included analysis of mean annual dose at 10^4 a, mean annual dose at 10^5 a, maximum annual dose for times up to 10^5 a, and performance measures for the vault, geosphere and biosphere (defined in Appendix D, Section D.5 and in Appendix E, Section E.3).

Iterated fractional factorial designs have been used to identify parameters that can be shown to have a significant effect on ADE and other consequences in SYVAC3-CC3 simulations. Although there is no conclusive proof that using this method (or any other method) can identify all the important parameters, we are confident in the results because

- Parameters are identified consistently using different groupings of parameters (including random selection of groups) and different sets of low and high values for the parameters.

- Parameters are identified consistently using both two- and three-level designs.

- The identity of important and unimportant parameters largely conforms with independent sensitivity analyses (using other methods). For example, there is good consistency between the results reported in Chapter 6 in the main text and the corresponding results documented in the primary references for the vault model (Johnson et al. 1994), the geosphere model (Davison et al. 1994) and the biosphere model (Davis et al. 1993).

- Reasonable explanations can be found as to why a parameter was identified as important (and why another parameter was not identified as important). The discussion on probabilistic sensitivity analysis (Section 6.5 in the main text and Sections E.4 to E.6 of Appendix E give many examples of such explanations.

Finally, we can obtain confirming evidence from supplementary sets of simulations. For instance, we can generate and then compare three sets of simulations:

- the original set, where all parameters are sampled randomly from their distributions;

- the "important" set, where only the important parameters are sampled randomly (and all other parameters are fixed at their median values); and

- the "unimportant" set, where only the unimportant parameters are sampled randomly.

The results of this comparison are discussed in Section E.3 of Appendix E. The discussion shows that, as expected, the original and important sets are nearly identical. Moreover, the variability in the results of the unimportant set is much less that the variability of the other two. These results provide further evidence that IFFD has identified all of the important parameters in SYVAC3-CC3.

While research effort continues for more powerful screening techniques, there is no doubt that IFFD is one of the best methods currently available for analysis of large computer models such as SYVAC3-CC3 (Saltelli et al. 1993, Andres and Hajas 1993).

A.4.3.2 Linear Regression Analysis

A standard method for analyzing variability in a data set is by multiple regression. This method assumes that there is a linear relationship between M independent variables, x_k, and a dependent variable, y. The mathematical form of the relationship is

$$y = a_0 + \sum a_k x_k + \varepsilon$$

where the summation runs over the M coefficients, a_k, that are to be determined, and where ε is a random error. The set of coefficients $\{a_k\}$ can be estimated by statistical analysis of N observations, N > M, where the set of x-values $\{x_{ik}\} i = 1,N$ and the y-value, y_i, are recorded for each observation. In linear regression analysis, the a_k are estimated by minimizing the sum of the squares of the deviations between the observed and predicted values of y. That is, linear regression analysis minimizes the sum:

$$\sum_{i=1}^{N} \left[y_i - y_i^P\right]^2 = \sum_{i=1}^{N} \left[y_i - \left(a_0 + \sum a_k x_{ik}\right)\right]^2$$

where y_i^P is the value predicted from the linear relationship.

The coefficient of determination, R^2, is commonly used to assess the fit; that is, to show how well the linear relationship explains the observed data. The definition of R^2 is

$$R^2 = \frac{\sum \left(y_i^P - \bar{y}\right)^2}{\sum \left(y_i - \bar{y}\right)^2}$$

where the summations are over N observations, and $\bar{y}$ is the average value of y_i. The coefficient of determination, R^2, may take on values from 0 to 1. A value of 1 means that all the variability in the set of points y_i can be explained by the linear dependence on the x_{ik}. A value of 0 means that none of this variability can be explained and implies that no such linear relationship exists.

The coefficient of determination has been used in the postclosure assessment to demonstrate that a large percentage of the variability of a parameter such as ADE can be accounted for by the set of important parameters identified by fractional factorial analysis. It has also been used to study the effects of using transformed data; for example, the logarithm of ADE has been examined to determine if its variability is more completely explained than the variability of the original (ADE) variable. (Section E.3.3.2 of Appendix E discusses why a logarithmic transformation is used.)

A parameter closely related to R^2 is the linear correlation coefficient, r_k, for a single parameter x_k. It is the ratio of the covariance between x_k and y and the square root of the product of the standard deviations in x_k and in y. Mathematically, r_k is defined as:

$$r_k = \frac{\sum_{i=1}^{N} \left(x_{ik} - \bar{x}\right)\left(y_i - \bar{y}\right)}{\left[\left(\sum_{i=1}^{N} \left(x_{ik} - \bar{x}_k\right)^2\right)\left(\sum_{i=1}^{N} \left(y_i - \bar{y}\right)^2\right)\right]^{1/2}}$$

where $\bar{x}_k$ is the average of the x_{ik}.

Correlation coefficients vary between -1 and 1. If a correlation coefficient, r_k, equals 1, then x_k and y are completely linearly correlated in a positive manner; that is, when x_k increases y also increases (and, by default, the other independent variables, x_j, have no effect on y). A correlation coefficient of -1 means that they are completely correlated in a negative manner; that is, when x_k increases y decreases. A coefficient of 0 means that x_k and y are not correlated; that is, when x_k increases, y may increase or decrease.

In the case of one independent variable (M = 1), the square of the linear correlation coefficient is equal to the coefficient of determination. The coefficient of determination applies to one or more variables, whereas the correlation coefficient applies to a single variable.

Correlation coefficients between single parameters and some dependent variable can be used to rank parameters. The larger the absolute value of the coefficient, the more important the parameter is known to be in influencing the dependent variable. (The converse is not true, however; parameters with a small correlation coefficient can also be important if there is a nonlinear relationship between x_k and y.) Linear correlation coefficients have been used, along with IFFDS, to rank parameters from SYVAC3-CC3 simulations. Numerous other methods exist for ranking parameters (Saltelli and Marivoet 1990, Saltelli and Homma 1992).

A.4.3.3 Confidence Bounds on a Regression Line

In this document, we include several figures showing scatter plots and regression lines to illustrate points about sensitivity analyses. Because the regression lines are estimated from the data, their positions and orientations are somewhat uncertain. To quantify the uncertainty for the reader, confidence bounds are placed above and below the regression lines. This section describes how to derive these bounds and what they mean.

Suppose we are given a data set containing N values of the form $\{(x_i, y_i)\}_{i=1,N}$. Because a scatter plot shows only two variables at a time, we have suppressed the second subscript k of x_{ik} used in the last section. We can draw a scatter plot of this data, as shown in Figure A-14. In the data set shown in this figure, there is a clear trend to the data: larger values of x correspond to smaller values of y.

Figure A-14 shows a straight line through the cluster of points, representing the least-squares fit described in the last section. That is, the line is so positioned that the sum of squared vertical distances between the line and the points in the data set is minimized. This line is known as a trend line or a regression line. It is the best fit to the data assuming that y and x are related by an expression of the form

$$y_i = a + bx_i + \varepsilon_i$$

where the ε_i's are random deviations.

Figure A-14 also shows two sets of curved lines:

- The dashed lines form a 95% prediction band around the regression line. This prediction band is defined such that for an arbitrary x value, x_i, the 95% confidence interval predicted for the corresponding y_i lies between the y-values obtained by intersecting the lower dashed curve and the upper dashed curve with the straight line $x = x_i$. *That is, the y_i should lie between the two bands 95 times out of 100.*

- The dotted lines form a 95% confidence band around the regression line. This confidence band is defined such that for an arbitrary x value, x_i, the 95% confidence interval for the mean y value, $\hat{y}_i$, is obtained by intersecting the two dotted lines with the straight line $x = x_i$. *That is, the true regression line should lie between the two bands 95 times out of 100.*

In summary, the dashed curves in Figure A-14 put bounds on individual observations (x_i, y_i), and the dotted curves put bounds on the location of the regression line itself. These latter curves are the ones shown on other scatter plots in this document.

Many of the expressions used in deriving expressions for these curves sum variables from 1 to N. The notation S_z will be used to represent the sum of the variable z_i from 1 to N. Thus

$$S_x = \sum x_i$$

$$S_y = \sum y_i \quad .$$

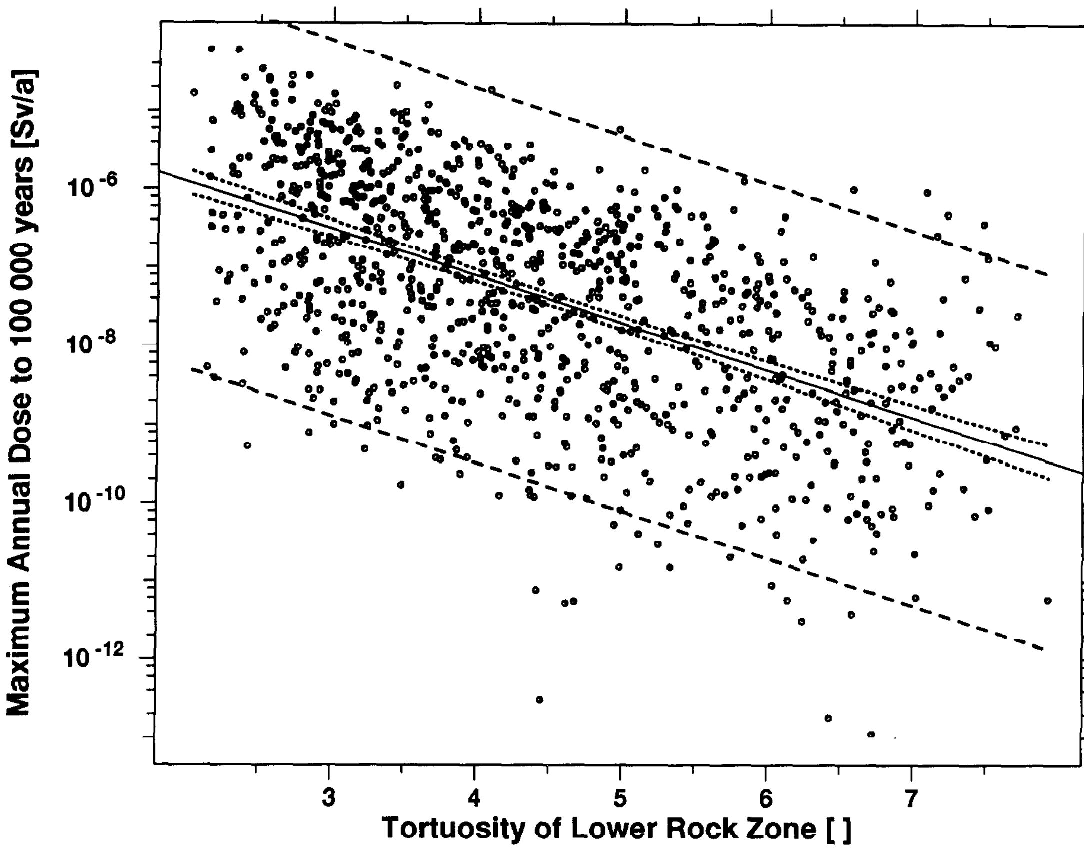

FIGURE A-14: Scatter Plot Showing 95% Prediction Limits and 95% Confidence Bounds

The tortuosity of the lower rock zone is the "X" or independent variable, and the logarithm of total annual dose at 100 000 a or the "Y" variable is dependent on it. The scatter of 1000 points randomly chosen shows a negative correlation; increasing X tends to reduce Y. The trend line minimizes the square of the vertical deviations.

The dashed lines form 95% confidence bounds on predicted values, so that about 95% of the points shown should lie between the curves. Very few points lie above the upper prediction limit, suggesting that errors may not be exactly normally distributed.

The dotted lines form a 95% confidence bound on the location of the "true" regression line. If an enormous number of points were sampled and a new regression line computed, the new line has a 95% chance of lying between the dotted lines at any X value.

Similarly, $\bar{z}$ represents the average value of the variable z. Thus

$$\bar{x} = S_x/N$$

$$\bar{y} = S_y/N \quad .$$

Scaled variables that have been shifted to have a zero mean will be represented with a prime:

$$x_i' = x_i - \bar{x}$$

$$y_i' = y_i - \bar{y} \quad .$$

Sums of products are shown with two subscripts:

$$S_{x'x'} = \sum x_i'^2 = S_{xx} - N\,\bar{x}^2$$

$$S_{x'y'} = \sum x_i' y_i' = S_{xy} - S_x S_y/N$$

$$S_{y'y'} = \sum y_i'^2 = S_{yy} - N\,\bar{y}^2$$

These identities are not obvious but may be readily proven.

Finding the least-squares fit to a data set is a matter of simple calculus. The objective is to choose a and b such that the sum of squares of ε_i's (that is, $S_{\varepsilon\varepsilon}$) is minimized. This technique is well-described in several books (such as Draper and Smith (1981)), and only the result will be described here.

The coefficients a and b that minimize $S_{\varepsilon\varepsilon}$ are given by the formulas

$$b - \frac{S_{x'y'}}{S_{x'x'}}$$

$$a = \bar{y} - b\,\bar{x} \quad .$$

This conclusion requires no assumption about the distribution of x nor about that of y; it is a straightforward solution to a minimization problem.

Putting confidence bounds about the regression line does require some assumption about the distribution of the residual errors, ε_i. Typically, these are assumed to be normally distributed with a mean of zero and with equal variances that can be estimated from the data. Barford (1967) presents a simple discussion of how normal errors can arise from the process of measurement.

The 95% prediction limits are curved lines, as shown in the figures, that enclose about 95% of the points. They are called prediction limits because, if we made one more independent observation of y_i at x_i, these limits form a 95% confidence interval for predicting where that observation would lie.

The other set of 95% confidence bounds shown in the figures lie much closer to the regression line. These bounds apply to the location of the "true" regression line, that is, the line we would get if we analyzed a set of observations of extremely large size.

To determine the prediction limits at some x_i, we need to calculate the standard error of y_i'', the predicted value of y_i. A standard error is the same in concept as a standard deviation, except that it applies to a derived statistic, such as a mean value or an estimated quantity, rather than a directly measured quantity. According to Sokal and Rohlf (1981), this standard error, denoted $s_{y''}$, is given by the following formula:

$$s_{y''} = \{(S_{y'y'} - S_{y''y''})[1 + (1/N) + (x_i - \bar{x})^2/S_{x'x'}](N - 2)\}^{0.5} \quad ,$$

where the sum of squared estimated values, $S_{y''y''}$, is evaluated from the following equation:

$$S_{y''y''} = \sum \left[y_i''\right]^2 = \left[S_{x'y'}\right]/S_{x'x'} \quad .$$

Because we had to estimate the expected value $\hat{y}_i$ and the standard error $s_{y''}$, we do not know the exact normal distribution that applies to each deviation ε_i. To correct for our uncertainty about the true mean and standard deviation of ε_i, we represent the distribution of ε_i by a t-distribution with mean zero, standard deviation $s_{y''}$, and N - 2 degrees of freedom. The t-distribution PDF has a similar shape to a normal density function, but it has more prominent tails. For N large (>>100), the t-distribution is virtually indistinguishable from a normal distribution.

To put lower and upper 95% confidence bounds on the estimated value, y_i'', we need first to find confidence bounds $z_{0.025}$ and $z_{0.975}$ on a t-variate with a zero mean and standard error of unity, having N - 2 degrees of freedom. (We use z_α to mean that quantile of the t-distribution having a cumulative probability value of α.) We want these particular quantiles so that the probability of a random value from the t-distribution lying between them is 0.975 - 0.025 = 0.95. By the symmetry of the distribution, $z_{0.025} = -z_{0.975}$. From published tables (Selby 1969), we obtain $z_{0.975} =$ 1.960 for large N, the same as for a normal distribution. For the y" t-distribution we are investigating, the 95% prediction limits are found at the points:

$$y_{0.95}(x_i) - a + bx_i \pm 1.960 s_{y''} \quad .$$

The same reasoning applies to finding the location of the 95% confidence bound on the regression line. The only difference is the calculation of the standard error. The standard error for the expected value of y at x_i is given by the following expression (Sokal and Rohlf 1981):

$$s_{\hat{y}} = \{(S_{y'y'} - S_{y''y''})[1/N) + (x_i - \bar{x})^2/S_{x'x'}]/(N - 2)\}^{0.5} \quad . \quad (1)$$

The 95% confidence bounds on the regression line are given by the expression:

$$y_{0.95}(x_i) = a + bx_i \pm 1.960 s_{\hat{y}} \quad . \quad (2)$$

A.5 MANAGEMENT OF COMPUTER RESOURCES

Most of the quantitative analyses described in this report make extensive use of modern computers and associated resources. We describe in this section some steps we have taken to manage these resources efficiently. We also describe the machines that have been used to run SYVAC3-CC3 and other codes used for sensitivity analyses of SYVAC3-CC3 results.

The discussion in Chapter 6 in the main text notes that 40 000 simulations have been performed for seven radionuclides and at least 2000 simulations for all other radionuclides and chemically toxic elements (Tables 5-3 and 5-4 of Section 5.9 in the main text list the contaminants of concern). We have found it convenient to examine the contaminants in small groups, each containing up to 10 contaminants, for three main reasons.

1. Results from a large set of simulations are available for analysis sooner. We frequently used results from a smaller number of simulations to initiate analysis and documentation. In addition, simulations for different groups of contaminants can be run simultaneously on different computers.

2. Storage space required to save the results is more easily managed. With all optimal outputs produced, SYVAC3-CC3 can produce computer files equivalent to hundreds of pages of results for a single simulation (most often used in tracing and checking intermediate calculations). For large sets of simulations, even more output can be generated, and we keep electronic copies of selected results for subsequent analysis. Typically, we would save data from approximately 8000 variables from 1 simulation involving 7 contaminants, so that 1000 simulations would require storage for 8×10^6 variable values. The use of small groups of contaminants reduces the amount of information stored from a single simulation or set of simulations, which in turn results in smaller electronic files. With the current limit of 10 contaminants in a group, the resulting electronic files are kept within a size and structure that can be reliably stored and accessed using our available computer resources.

3. We can perform more simulations dealing with the contaminants contributing most to risk. In the analyses documented here, we have examined 11 groups of contaminants. Each group was ranked, and we first performed simulations for those groups that we expected would result in the largest radiological and chemical impacts. We then performed more simulations for those contaminants that we observed contribute most to the radiological risk. In the assessment of the reference disposal system, 40 000 randomly sampled simulations were performed for seven radionuclides (including ^{14}C and ^{129}I) that most contributed to estimated radiation doses.

Our method of analysis includes some additional considerations that permit the above resource management plan. For example, results from different sets of simulations can be combined because

- We employ simple random (Monte Carlo) sampling, so that results from two different sets of 1000 probabilistic simulations can be combined to give results from 2000 probabilistic simulations.

- We use carefully selected random number seeds to initiate different sets of probabilistic simulations. These seeds are chosen so that a unique collection of parameter values is associated with each and every probabilistic simulation for a single group of contaminants. For instance, suppose that we wish to run ten sets of 10^3 simulations, and each simulation requires about 10^4 randomly sampled numbers. Thus each set of simulations will require about 10^7 random numbers. We use a scheme in which each set of simulations has a reserved initial seed, and each seed can generate its own "special" stream of 10^7 random numbers. These streams of random numbers are "special" in the sense that any random number can appear once, and only once. That is, each stream of numbers is mathematically disjoint, meaning that no random number is reused.

  The foregoing description is a simplification; we actually reserve several initial seeds and their associated random-number streams to generate the required collections of random numbers. One such initial seed would be used exclusively for contaminant-dependent parameters. As a result, we can arrange the randomly sampled simulations for each of the 11 groups of contaminants so that they use the identical sequence of (randomly selected) parameter values, except for contaminant-dependent parameters. This produces equivalent results to performing the same set of simulations but involving all contaminants at one time.

- We use the probabilistic simulations to estimate the arithmetic average of the annual dose (Section 6.5.1 of the main text). This parameter is additive: the arithmetic mean doses attributed to different radionuclides can be added to give their total mean dose, and arithmetic means from two different sets of probabilistic simulations can be added to get a mean for both sets.

In addition, SYVAC3-CC3 is re-startable. Thus we could efficiently continue a large set of simulations when they were halted because of problems such as a power outage.

Computer codes used in this postclosure assessment include the main simulation code, SYVAC3-CC3, and software used in the analysis of SYVAC3-CC3 results, such as SAMPLE (Andres 1987) for sensitivity analysis using IFFD, WRKOUT (Bera and Hajas 1993) to extract selected results and perform simple statistical analyses, and S (Becker et al. 1988) to perform more sophisticated data manipulation and statistical and graphical analyses.

For the most part, these codes have been run on Digital Equipment Corporation Virtual Address eXtension (VAX) computers. We have used both mid-sized computers such as the VAX 6620, and compatible workstations such as the VAX 3100 M76. Execution of SYVAC3-CC3 was normally carried out in batch mode, and Table A-3 gives examples of its execution time and storage

TABLE A-3

TYPICAL COMPUTER RESOURCE REQUIREMENTS FOR SYVAC3-CC3

Number of Simulations	Execution Time* for VAX Computers mid-size	micro	Typical** Storage Needs for Output
1	17 m	25 m	10.5 megabytes
1000	40 h	160 h	26.5 megabytes

* Each execution of SYVAC3-CC3 requires some overhead time to read in and check the input files, so that the computing time required to process 1000 simulations is not 1000 times the time for one simulation.

** For one simulation, information typically stored includes results used for a detailed study of intermediate calculations. For 1000 simulations, information typically stored is the final set of results for approximately 8000 variables from a group of seven radionuclides.

requirements. For typical computer loads at the Whiteshell Laboratories, results would be available within an hour of submission for a single simulation and within several days for 1000 simulations. Computer codes used to analyze results from SYVAC3-CC3 are typically run in the interactive mode.

Other computer hardware used with our analyses include microcomputers running MS-DOS[R] (Microsoft 1991) and a variety of peripheral devices. We required fast and reliable access to large volumes of electronic information because, as noted earlier, SYVAC3-CC3 typically stores results from 8000 variables for each of up to 40 000 simulations. Our associated computer hardware includes conventional magnetic-disk storage devices controlled by VAX computers, and more recent magneto-optical disk storage devices controlled by VAX workstations.

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APPENDIX B

QUALITY ASSURANCE OF MODELS, DATA AND COMPUTER SOFTWARE

CONTENTS

continued...

CONTENTS (concluded)

B.1 INTRODUCTION

Quality assurance (QA) is the system of means and actions to provide confidence that a given product meets requirements and performs its intended functions satisfactorily. Quality assurance is important to the postclosure assessment of nuclear fuel waste disposal because the assessment involves complex models of extensive natural and engineered systems, many uncertain and variable parameters, and large computer codes. In addition, the results of the assessment may influence decisions with large financial and significant safety implications.

The QA program was developed in parallel with the postclosure assessment project. It has matured following an iterative and evolutionary procedure, using feedback from interim assessments for continuous improvement. What has remained constant in the QA program are its major features and objectives. An improved program and high-quality products can be expected once site-specific studies are initiated, mainly because a complete and mature QA program will be in place from the beginning of the project.

The discussion in Section B.2 outlines the QA program for the postclosure assessment documented in this report. Section B.3 describes in more detail the quality assurance procedures used in the development of the SYstems Variability Analysis Code, generation 3, using models for the Canadian Concept, version 3, for the disposal of Canada's nuclear waste (SYVAC3-CC3). That is, it documents the measures taken to show that the code correctly implements the systems variability analysis approach and the CC3 system model.

Documentation on the justification and applicability of the CC3 models and data is contained within the primary references for the vault model (Johnson et al. 1994), the geosphere model (Davison et al. 1994) and the biosphere model (Davis et al. 1993). We include in this appendix a discussion of comparisons that have involved the computer code SYVAC3.

- Section B.4 discusses the credibility of the models used in SYVAC3-CC3 for the postclosure assessment of the reference disposal system. It provides evidence that the models and code properly represent the physical features and behaviour of the Concept for disposal of Canada's nuclear fuel waste for nuclear fuel waste disposal.
- Section B.5 describes the quality assurance procedures pertaining to the data used in SYVAC3-CC3 for the postclosure assessment of the reference disposal system. It provides a clearly defined trail showing how the data specified for the postclosure assessment is supplied to SYVAC3-CC3.

B.2 THE QUALITY ASSURANCE PROGRAM FOR THE POSTCLOSURE ASSESSMENT

The objectives of the quality assurance program for the postclosure assessment discussed in this report are

- to demonstrate compliance with regulatory safety requirements, notably those stated by the Atomic Energy Control Board (AECB) (1985, 1987);

- to increase confidence in the assessment, especially with regard to concerns of safety for the public and the environment; and

- to contribute to the verification and (to the extent possible) the validation and evaluation of assessment results.

Validation is commonly regarded as a procedure that involves comparison of the predictions of a model with observations of a real system. In the case of the postclosure assessment, the results from SYVAC3-CC3 apply to times up to 10^4 a and longer. This implies that validation cannot be achieved in full because the operation of an actual disposal system cannot be observed over the time frame required to permit comparison with results from SYVAC3-CC3. There is also no direct analogue known in nature that would permit a complete comparison. Nonetheless, different components of the model may be validated to some extent, through comparisons with experimental observations (generally covering short times spans) and with natural analogues (often covering long time spans).

Complete validation of the models contained in SYVAC3-CC3 is, therefore, not achievable. However, Dormuth (1993) notes that validation is not essential:

> ...it is not generally necessary to show that performance-assessment models make accurate predictions of actual performance. Rather, it is necessary to answer the following: given an analysis employing, in general, a mathematical model, computer program, data input, numerical results, and interpretation of results, is the conclusion justified by the analysis? The answer to this question may or may not require model evaluation by comparison with observations. For example, in safety assessments it is sometimes necessary to establish only that the impacts are likely to fall below a quantitative safety criterion. In such cases, models may err on the side of conservatism or bound the impacts. In fact, it could be satisfactory or desirable to use a model that is not realistic, and not subject to validation, as long as it overestimates the impacts.

In contrast to model validation, model evaluation is feasible. Model evaluation is defined as the

> activity of assessing the reliability of a model through observations of real systems. No level of accuracy is specified beyond which a model itself is considered to be validated. Instead, the information from the model evaluation is used by assessment analysts to help establish confidence in their performance assessments. A model that has been compared with observations is said to be evaluated, and the more thorough a set of observations the model has been compared with, the more thor-

> oughly evaluated it is. Saying that a model is evaluated does not in itself mean that the model is suitable for a particular application. Deciding that the model is suitable for an application is a judgment that must be made with a knowledge of the requirements of the application and information about the characteristics of the model, including information from any model evaluation that has been done (Dormuth 1993).

Similar views are expressed by McCombie and McKinley (1993), who state that the validity of a model depends upon the complexity of the system being modelled, the use of the model, and what accuracy and degree of confidence is required in drawing conclusions about possible consequences of reasonable evolution scenarios.

Our QA measures are, therefore, designed to provide confidence in the reliability and credibility of the results reported in this postclosure assessment, with an emphasis on model evaluation rather than model validation.

The QA program deals with all phases of the postclosure assessment life-cycle: planning, research, model development, code development, computer simulations and analysis of results. It incorporates the concept of "built-in" quality, with emphasis on defect prevention and correction. Quality attributes are defined and priorities established, particularly for software. Attributes such as reliability, understandability, usability, completeness, and efficiency are considerations in the work procedures (see Section B.3 and IAEA (1987) for an extended list and for definitions of software quality attributes).

The QA program addresses work organization, qualification of personnel, effectiveness of procedures, control of products and review of documentation.

B.2.1 WORK ORGANIZATION

The postclosure assessment and development of the associated computer codes are the responsibility of the Environmental and Safety Assessment Branch and, in particular, the Postclosure Assessment and Software Development Sections, working cooperatively and in close communication with each other. The project is divided into functional areas for the executive, vault model, geosphere model, and biosphere model, with specialty teams assigned to each area. Regular project meetings are held to discuss plans, progress, and problems; frequent direct communication occurs among all involved staff.

For each of the three major models of the disposal system, a Model Working Group has the responsibility to define and justify the assessment model and the data. Each Model Working Group includes a representative from the Environmental and Safety Assessment Branch who is responsible for development of the associated model in SYVAC3-CC3. Each Group also has representatives from research and development organizations across the CNFWMP, with responsibilities for the scientific and engineering expertise required to support the CC3 model.

Other special projects, such as scenario analysis, involve task groups whose members are selected from all appropriate research disciplines within the CNFWMP.

B.2.2 QUALIFICATION OF PERSONNEL

Postclosure assessment staff have post-secondary education and experience in a wide variety of fields that are pertinent to the waste disposal system, including computer science, mathematics, chemistry, physics, geology, biology and engineering. The varied backgrounds of the staff, who work closely together, contributes to the elimination of errors in models, data and code. In addition, many members of the group have taken specialized training in modelling techniques, numerical analysis, structured analysis, design, coding, and testing of software, as well as project management. To keep up to date on methods, conferences and symposia are attended regularly.

B.2.3 EFFECTIVENESS OF PROCEDURES

Many of the activities performed for the postclosure assessment are controlled using documented procedures. For example, procedures have been established for

- the translation of mathematical and scientific models to computer software using model and design specifications;

- the movement of data from its source to the input files used by SYVAC3-CC3 using a master database;

- the submission of SYVAC3-CC3 for execution on a computer, including control of input files and output files; and

- the development of FORTRAN software following specific standards (such as those described by Hoffman and Sherman (1985)).

These procedures are periodically reviewed and refined, to improve their effectiveness as elements of quality assurance and quality control.

B.2.4 CONTROL OF PRODUCTS

Computer software items produced to support the postclosure assessment are under strict control. This control includes

- *Access to critical files.* Each such file can be modified by only one authorized individual. Critical files include those that store the FORTRAN code making up SYVAC3-CC3, those that contain the data used by SYVAC3-CC3, and those containing results of the simulations.

- *Independent development and inspection of products.* The development and preliminary testing of software is performed by one or several individuals, and a different group of individuals is responsible for inspection, review, and approval of the resultant computer software products.

- *Records describing all changes to computer software products.* All changes are documented on a standardized form, recording the reasons for the change, the items produced (such as new specifications and new code files), the personnel who performed the work, including who tested, inspected, reviewed, and approved the change, and the date of completion of each stage of work.

- *Records describing all data used in the simulation.* All data used in SYVAC3-CC3 are stored in computer files. These files include a full description of the data, identification of the personnel who authorized its use, and a brief justification of its choice. Access is fully controlled so that only one authorized individual can write to or modify these files, although other personnel in the program can examine the information they contain.

- *Systematic release of reference versions of computer software.* Each version is uniquely identified, and the collection of products comprising a complete computer code are stored together in computer files with an associated written record (the latter includes the completed change forms). The collected products are archived and have controlled access.

B.2.5 REVIEW OF DOCUMENTATION

AECL has established a formal review and approval procedure for all publications and documents it releases. The review process typically involves detailed examination of documents by one or more scientists and engineers who have an appropriate level of expertise. Approvals are required by line management before a publication can be released. Finally, many externally published reports undergo a further level of peer review, organized by the publishers.

All simulation results appearing in the postclosure assessment are also reviewed in detail. This review includes confirmation that data referenced in the text, in tables, and in figures are correct. The process of extracting and manipulating SYVAC3-CC3 output data is repeated by a person other than the one who originally did the work. The use of graphical and data analysis tools, computer command procedures, and the specific data files used are recorded and archived, along with the computer procedures and scripts employed.

B.3 SOFTWARE QUALITY ASSURANCE

B.3.1 INTRODUCTION

The SYVAC3-CC3 computer program is used for preparing quantitative estimates of impact for the postclosure assessment study documented in this report. It has been developed over a period of about ten years. The previous generations, SYVAC1 and SYVAC2, were used to perform interim assessments (Wuschke et al. 1981, 1985; Goodwin et al. 1987); both the codes and assessment results have been widely reviewed and commented upon by the scientific community.

The software and its development procedure have been externally reviewed throughout the development period. This includes review (although not necessarily endorsement) by the Technical Advisory Committee on the Canadian Nuclear Fuel Waste Management Program (TAC 1993 and preceding reports) and the AECB. Several international waste management organizations are actively using and developing their own versions of SYVAC (including the U.K. Department of the Environment, the U.S. Department of Energy, the Swedish National Board for Spent Nuclear Fuel, and the Spanish waste management agency). There has been useful cooperation with and feedback from these organizations, including detection and subsequent removal of defects. Finally, parts of SYVAC3-CC3 have also been used in code intercomparison exercises of the Nuclear Energy Agency (NEA) of the Organisation for Economic Cooperation and Development (OECD) (see Section B.4).

Other software has contributed to the postclosure assessment, but quality assurance efforts have been concentrated on SYVAC3-CC3 because it most directly affects the assessment. Supporting software has been subjected to many of the quality assurance measures described below.

The software QA program under which SYVAC3-CC3 has been developed has evolved over the project lifetime. What is described here is the current state of the program. Actual practices may not have been entirely as described for every piece of the software. However, the objectives have not changed; although techniques may be different, there has always been the intent to produce high-quality products.

B.3.2 ELEMENTS OF SOFTWARE DEVELOPMENT

Software development is based on accepted principles of sound software engineering practice, integrated with QA principles. The development framework takes into account the following considerations:

- specified priorities for software quality attributes,
- standards and conventions,
- development methods,
- configuration and change control,
- verification, review and approval, and
- application of automated software development tools.

These considerations are described further in the sections that follow. They are applied to the software development functions of analysis, design, coding, testing and documentation, and the QA activities of planning, control and verification. They are performed by staff whose education and experience is commensurate both with software development and with the technical aspects of the disposal system.

B.3.2.1 Software Quality Attributes

The list of desirable software quality attributes is very long; IAEA (1987) shows a sample list. However, many attributes are very similar or encompassed by others, thus we have chosen to concentrate on nine attributes for SYVAC3-CC3. The goal is to best achieve these attributes, recognizing that some are contradictory so that judgment is needed to obtain a balance leading to the highest overall quality. For example, usability, or the ease of operating the program, may be increased at the expense of completeness or the number of options available, or portability could be increased by coding practices that reduce the efficiency on a particular system.

A description of the nine selected attributes follows.

Reliability

- The ability to produce, from specified input, specified outputs that are sufficiently precise to satisfy their intended use; and
- The extent to which specifications are satisfied and the code can be expected to continue to perform its intended functions.

Understandability

- The clarity of the functions of the software, as determined by its use of standard control structures, simplicity, conciseness (minimum repeated code but not excessively fragmented), consistency in format, notation, and structure, and communicativeness (comments, meaningful mnemonics, clearly annotated inputs and outputs).

Usability

- The effort required to learn, operate, prepare input and interpret output;
- The flexibility allowed in input, functions performed and data storage; and
- The help provided to the user who may encounter errors resulting from input, hardware or software.

Completeness

- The extent to which all required functions are present, developed and documented; and
- The availability of information required to determine or verify objectives, assumptions, constraints, inputs, outputs, components and development history.

Maintainability

- The ease with which additions and revisions can be made.

Portability

- The ability to be moved and to operate well on different computer configurations; and

- The independence from computer operating systems, hardware and peripheral equipment.

Testability

- The extent of facilitating establishment and implementation of test plans, specifications and procedures.

Reusability

- The ease with which the program in whole or in part can be interfaced to other programs and used in other applications.

Efficiency

- The economy of computer resource requirements to run the program, particularly processor time and storage space.

B.3.2.2 Standards and Conventions

Many standards and quality assurance guidelines were considered in the planning of the software development process, including several from the Canadian Standards Association (CSA 1982a, 1982b, 1985, 1988, 1990), the Institute of Electrical and Electronic Engineers (IEEE 1983a,b; 1984a,b; 1986a,b, 1987), the North Atlantic Treaty Organization Allied Quality Assurance Program (NATO 1981), the International Atomic Energy Agency (IAEA 1978, 1979, 1983, 1984, 1987), the United States Department of Defence (US DOD 1988a,b), and the American National Standards Institute (ANSI 1978; 1986a,b; 1987; 1988; 1991). The software development process that was followed is not based on any one specific quality assurance standard, but the principles were adopted in a form applicable to scientific research purposes, where:

- The requirements and expected results may not be well known from the outset, and

- A large number of revisions have to be made rapidly, as results are examined and the general knowledge base increases.

Project-specific standards and conventions for the format and contents of software products follow the updated recommendations of Hoffman and Sherman (1985). For example, FORTRAN-77 standards (ANSI 1978, 1991) are used for the code, with the following designated exceptions:

- lower case is permitted in comments and literal text output;

- the exclamation mark comment indicator may be used in the variable description section of the code;

- the IMPLICIT NONE statement is included in each module; and
- the INCLUDE statement is used to insert FORTRAN PARAMETER specifications, COMMON statements, and declarations of the associated variables.

These exceptions are allowed because of the substantial advantages they provide, while being easily and automatically convertible to standard FORTRAN-77 code. Readability and understandability of the code and output are enhanced through use of lower case to help distinguish between comments and executable code. Use of the exclamation point comment indicator allows the definition and units of each variable to be provided in a compact and easily recognized form, providing the maximum amount of information in each display screen. The IMPLICIT NONE statement enforces declaration of each variable, thereby reducing data typing errors and detecting misspelled variable names. The INCLUDE statement helps avoid repeated code and reduces the effort and risk of error associated with modifying all instances of duplicate code.

Conventions are also followed for the naming of files and computer disk directories. This is helpful in distinguishing file contents and versions, and program structure and function. These conventions are compatible with the file access protection system, for maintaining control and assigning individual responsibility for each software item.

B.3.2.3 Development Methods

Structured techniques are used for analysis, design and coding. Although no single software development methodology is used, the methods of Yourdon (1979, 1982) and DeMarco (1979) have had the greatest influence. Some influence from Martin and McClure (1985) is also apparent in the form of the software products (these products are outlined in Section B.3.3).

B.3.2.4 Configuration and Change Control

Responsibility for each software product is assigned to specific individuals, and a documented scheme is used to store the products. Figure B-1 shows an example: it is a copy of the change request form used to track software development. For each step in the development process, it lists the software items and personnel involved, including identification of personnel responsible for reviewing and approving the activity.

Configuration control for SYVAC3-CC3 uses the well-established file directory structure and access protection of the Digital Equipment Corporation VAX-VMS operating system. Software products are stored in hierarchical directories, segregated according to the major functional parts of the software (executive, vault model, geosphere model and biosphere models, and packages within them, such as parameter sampling and time-series management), and the software development step producing them. There are also separate directory structures for various versions of the software, including released versions and the current development version. Version identification is embedded in the directory names. Backups of each version are kept physically separate and secure on optical disk and magnetic tape.

Number:________

SOFTWARE CHANGE REQUEST

LIBRARIANSHIP

Submitted by: Date:

Version number of the division(s) affected:
SV3___ ML3___ CC3___ SUP___ TLS___ CFG___ Other_________
Packages or Programs affected:

Modules affected:

Description of the change or problem: (attach if necessary)

Change description summary (for folder records file):

Recorded by: Date:

ANALYSIS

Analysis by: Date:

Comments / Names and versions of analysis products:

Functional Test Data: not required [ ] or attached [ ]

Approved [ ] with priority ____, or terminated [ ](give reason above)

IMPLEMENTATION

Implemented by: Date:

Comments / Names and versions of implementation products:

Implementation completed [ ], or terminated [ ](give reasons above)

90-APR-05 Form ESAB-CR-3B (continued over)

Number:________

INSPECTION

Inspection by: Date:

Comments (attach if necessary):

Inspection completed [ ], or terminated [ ](give reason above)

INTEGRATION

Integration by: Date:

Run request number _________
Comments / Names and versions of integration products:

Integration completed [ ], or terminated [ ](give reason above)

REVIEW

Review by: Date:

Comments (attach if necessary):

Approved for installation [ ], or terminated [ ](give reason above)

INSTALLATION

Computer files installed by: Date:

Paper files installed by: Date:

Version number of the division(s) installed into:
SV3___ CC3___ ML3___ SUP___ TLS___ CFG___ Other_________
Comments:

Installation completed [ ], or terminated [ ](give reason above)

90-APR-05 Form ESAB-CR-3B (concluded)

FIGURE B-1: A Change Request Form for SYVAC3-CC3 Software

One of these forms is used to control and track each software change to SYVAC3-CC3, including addition of new software. The form is sectioned according to the different steps in the software development process and is passed sequentially to those individuals who are responsible for the completion of each step. At the conclusion of each step, there is a review and formal sign-off, indicating that all required activities have been completed and that all required documentation has been produced.

Each part of the software is comprised of many files for design, documentation, code and testing. The FORTRAN code making up SYVAC3-CC3 is broken into about 665 modules, and each module is a small stand-alone unit of software, such as a subroutine or COMMON block. All modules are stored in separate files, named using the module name. Embedded in each file is information on the name and purpose of the module, and a history of version numbers, the date of creation and identification of the authors.

Access to all SYVAC3-CC3 files is controlled in two ways:

- The normal file protection mechanism offered by the VAX-VMS operating system. Using this mechanism, execute, read, write and delete privileges can be selectively assigned to different groups of users who have access to the computer.

- Access control lists, to provide more specific protection. Different levels of access privilege can be assigned to specific individuals. SYVAC3-CC3 files and complete directories of files are regulated such that most individuals can only read and execute the files. The capability to write and delete files is strictly limited to authorized personnel. Only authorized individuals have the authority to change particular files; they also have responsibility for the content of the files.

B.3.2.5 Verification, Review, and Approval

The software development process incorporates specific inspection and review steps, and includes unit, functional and system tests (see Section B.3.3 and Figure B-2). Each step requires formal approval, and the work is scrutinized as it is used by the succeeding step. There is provision for iteration through the steps in the event that any deficiencies are detected.

B.3.2.6 Automated Software Development Tool Application

Several commercial and many locally developed tools are used to automate the software development process (making it less prone to human error) and to provide checks. These tools include code generators, static and dynamic code analyzers, documentation generators, and character, graphics and word processing editors. Table B-1 lists some of the tools used during the development of SYVAC3-CC3.

B.3.3 THE SOFTWARE DEVELOPMENT PROCESS

All SYVAC3-CC3 software development is considered to be a change, including the addition of new code. The process is initiated when a user or developer submits a change request form (shown in Figure B-1) to the software project librarian.

Figure B-2 illustrates the series of elements or steps that make up the SYVAC3-CC3 software development process. Most elements are performed sequentially for each change made to the code, and several are completed periodically. These elements integrate software production and quality assurance activities. A system for control of the software configuration (and change) is also closely coupled with the development process.

TABLE B-1

EXAMPLES OF SOFTWARE DEVELOPMENT TOOLS USED IN THE DEVELOPMENT OF SYVAC3-CC3

Name	Purpose
ADDFR	add a folder record—to record the status of software changes.
CHEKER	FORTRAN coding convention checker—to promote consistency in coding style.
DDMERG	data dictionary merge—to combine lists of variable definitions.
DECdesign	Digital Equipment Corporation analysis and design tool—used for the production of data flow diagrams.
DSTRUC	analyze and document the data flow and call structure of FORTRAN code.
FPE AUDITOR	FORTRAN Programming Environment Auditor (Softool Corporation)—for static syntactical analysis of code.
PCA	Performance and coverage analyzer (Digital Equipment Corporation)—to determine and record the extent to which the code is exercised during testing.
RESEQ	resequence FORTRAN statement labels—re-number the labels so that they appear in order and at equal intervals.
STRCHT	draw a program structure chart.
UNITCK	physical unit checker—analyzes the balance of physical units of variables in FORTRAN expressions.

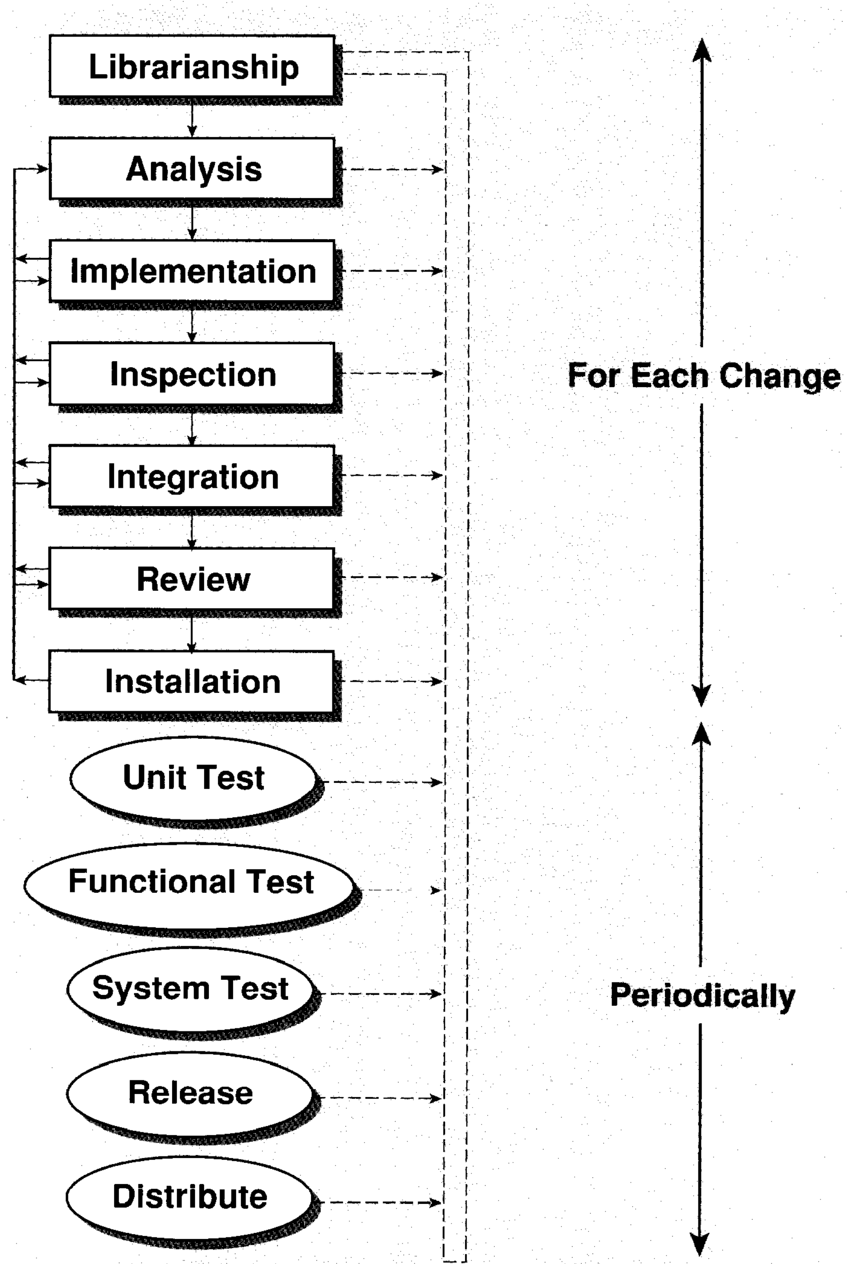

FIGURE B-2: The SYVAC3-CC3 Software Development Process

A sequential set of steps, shown as rectangles, are followed for each change. The sequence is indicated by the arrows leading from one rectangle downwards to the next. There is provision for feedback to previous steps in case deficiencies are found, as indicated by the arrows on the left of the rectangles. Each of these steps contributes to the librarianship function, as indicated by the dotted arrows on the right-hand side of the rectangles. In addition, several functions, indicated as ovals, are performed periodically.

Each element in Figure B-2 is briefly described below, with emphasis on quality assurance aspects.

B.3.3.1 Librarianship

This function begins the configuration and change control process and the creation of a change audit trail. Each change request form is assigned a number and placed in a file folder. This folder is passed to each person involved in the development process. Additional material is added to the folder; for example, documents produced during development, records of all work done and official approvals given at each step in the development process. At the installation step (Section B.3.3.7) in the software change process, this folder and its contents are filed by the project librarian and provide a permanent record of actions taken during processing of the change.

In addition, each change request is tracked by an entry in a computer data file that records the submission information. This entry is supplemented at each step of the development process to provide up-to-date information on the status of all the change request.

B.3.3.2 Analysis

The main purpose of the analysis step is to document the function to be coded and to identify essential function-specific data (that is, data central to the problem rather than those required only to implement a particular solution). This documentation uses notation that is suitable for the subject area of the problem addressed, easily understood by experts in that field, and is reviewed by some of these experts. Use of data flow diagrams, data dependency diagrams and data dictionaries is encouraged. In addition, other means are used if they are more effective, such as a synopsis containing mathematical equations with accompanying written descriptions.

The analysis function also provides data values to be used both in functional tests of the code produced and in the expected results from that data. Further, a priority for implementation of the change is assigned so that related or dependent activities can proceed in a logical manner.

B.3.3.3 Implementation

Implementation is divided into four parts that can be done iteratively for different parts of the change:

- *Design.* The purpose of software design is to define and document the code structure, logic and detailed transfer and storage of data. For revisions to existing code, it also provides a user-oriented description of the change. Documentation produced by the design step includes program structure charts, algorithm specifications (such as pseudocode), file and COMMON block descriptions, templates for user supplied modules and data dictionaries.

- *Code.* Source language files are created or revised, as are code data dictionary files.

- *Check.* To ensure code consistency, static analysis tools are applied to all source code. These tools include codes that perform syntax analysis, check compatibility with format standards and test for consistency in physical units of variables in all applicable source code statements.

- *Debug.* Code is compiled and linked in functional units of each major model. Several test cases are simulated, with data that are typical and that one data selected to exercise portions of the code judged to be potentially most troublesome. Complete code coverage is not required (compare with Section B.3.3.8), but tests are instrumented to report which statements were exercised in the tests.

B.3.3.4 Inspection

To obtain an independent check with a different perspective, the implementation products are inspected by personnel other than those who carried out the implementation. Inspection is usually completed by the analyst responsible for the code involved. The word "inspection" as used here is not meant to imply the formal process described by Fagan (1976), but rather the common dictionary meaning, more akin to "code reading" and "desk checking," and includes examination of the test results produced by the stand-alone model tests done in the implementation step.

B.3.3.5 Integration

This step integrates the revised code into a complete program. Minor code changes (ones that are not expected to affect the code function, such as modification of comment statements) may be made if necessary for the integration or to comply with formatting standards. All such changes are documented. The complete code is compiled and linked, and then tested.

B.3.3.6 Review

The analyst responsible for the new code reviews the previous work, particularly the integration and integration test results, to ensure that the objective of the change has been met and that the change has been made in a suitable fashion. If the code change necessitates a change to the reference input data, an associated database change request is issued.

B.3.3.7 Installation

Computer files produced throughout the development process for each change are copied from development directories to the current reference directories. This step contributes to configuration control because these reference files can be created or deleted only by an authorized individual.

All relevant documentation associated with the change, including the completed change request form, is filed by the project librarian. A copy of the completed change request form is sent to each person involved in the change, as notice that the installation is complete.

B.3.3.8 Unit Testing

Testing at the unit (or individual subroutine) level is done to check the software at the most detailed level and to achieve complete test coverage. Visual inspection of the design documents and code is done using checklists to identify desirable attributes and typical error-prone constructions. Driver programs and stubs for called modules are written to execute individual modules. Test data are prepared and expected results determined. Test simulations are then done, ensuring that every statement in the test module is executed, and then the expected and actual results are compared. The test process is documented and all pertinent documentation and files are archived.

Unit tests are initiated at the direction of the project manager, usually when a reasonably stable program is achieved. Kersch and Oliver (1994) describe unit testing of some SYVAC3-CC3 modules, performed by contractors for the United States Department of Energy.

B.3.3.9 Functional Testing

Functional testing concentrates on groups of modules and their operation together to perform more general functions than individual modules. Some of this type of testing has already been done during development and is supplemented in this step by using additional data sets. Emphasis is on critical or suspect functional units of code and on previously untested options and conditions. As with unit testing, these tests are fully documented and all pertinent files are archived.

Functional tests are initiated at the direction of the project manager, usually when a reasonably stable program is achieved.

B.3.3.10 System Testing

To check all module interfaces and ensure that the general objectives of the complete program are met, the integrated program is tested in a systematic way using sets of data that exercise every major program function and option. Documentation includes matrix charts relating the function tested to the test data set used. All pertinent material is archived.

System tests are initiated at the direction of the project manager, usually when a reasonably stable program is achieved.

B.3.3.11 Release

Release provides a reference version of the code for subsequent use. A collection of static analysis and documentation tools are run on the version to be released.

The access protection of the released version is changed so that only the project leader has the ability to change or delete the files. No further changes are made to the software in these directories.

A copy of the released version is moved into directories to be used in future development.

B.3.3.12 Distribution

Distribution involves setting of a unique serial number in the source code and making copies of both electronic and paper material. Records are kept of what material is sent to whom and when.

B.3.4 SUMMARY AND CONCLUSIONS

The software QA program for the postclosure assessment has clear objectives, with reliability being foremost, and it includes many other important software attributes. The organization of this quality program is aligned with the function to be performed and makes use of the extensive skills and expertise of the staff involved. Specific, detailed procedures guide each task. Many concepts of quality are addressed: to build in quality during the routine production tasks, to provide products fit for their intended use, and to give confidence in their use.

B.4 MODEL QUALITY ASSURANCE

B.4.1 INTRODUCTION

Much of the postclosure assessment relies on mathematical models that are implemented in a computer code, SYVAC3-CC3. They are used to simulate features, events and processes that could lead to the escape of radionuclides from the disposal vault and to provide bounding estimates of subsequent effects for thousands of years after closure of the vault. Because the simulations are projections of events far into the future, a direct comparison of estimated impacts with observations (or model validation) is not possible. Hence, as noted in Section B.2, we use a series of model evaluations to help establish confidence in the models utilized in the postclosure assessment.

The models used in SYVAC3-CC3 are generally condensations of detailed research information and contain the essential features needed for the assessment simulations. They were constructed through the efforts of three Working Groups, one each being responsible for the vault, geosphere, and biosphere models that make up the system model. These same Groups were also responsible for documenting the evaluation support for the models, provided in the primary references for the vault model (Johnson et al. 1994), the geosphere model (Davison et al. 1994) and the biosphere model (Davis et al. 1993).

Our discussion is focussed on measures that give credence to the successful implementation of the models in the SYVAC3-CC3 code. Two types of activities have proven particularly useful:

- comparisons of sample simulation results with those produced independently by other groups, and

- analysis of the sensitivity of the assessment results to changes in the models and data.

These activities are described in the following sections. Another powerful activity, comparisons with observations of natural analogues, is documented in separate reports (Cramer 1986, 1993; Goodwin et al. 1989).

B.4.2 COMPARISON WITH MODELS DEVELOPED BY OTHER GROUPS

One method of building confidence in SYVAC3-CC3 is through comparisons of results from similar computer codes. Such comparisons are particularly useful if they involve codes that have been independently developed to treat the same problem:

- Similarity in the models used and the structure of the codes provides evidence that a common understanding exists concerning the processes of importance in the system and the way in which they should be modelled.

- Similarity in the estimated impacts and identification of important processes and parameters increases our confidence in the models and codes.

Several groups throughout the world are engaged in assessment work for radioactive waste management (AECL 1994). Thus there is a variety of models and data under development for use in simulating nuclear waste disposal systems. Some of the associated cooperation and interaction between these groups is discussed below.

B.4.2.1 Comparisons with NUTP

One achievement of the Canadian National Uranium Tailings Program is a computer code called UTAP (for Uranium Tailings Assessment Program). The UTAP environmental assessment code simulates the movement of radionuclides and chemically toxic elements away from a pile of uranium mine tailings (SENES 1985, 1986; Holmes 1987). AECL Research was contracted to

- carry out an independent development of the specifications for the tailings model;

- produce the corresponding code, based on SYVAC3; and

- simulate the same scenario as that for the UTAP code.

The results of these studies show acceptable agreement between the results produced by the UTAP code and the code based on SYVAC3 (Goodwin and Andres 1986, Goodwin et al. 1987), thus generating confidence in both codes.

B.4.2.2 Comparisons with PSAC

Several assessment groups that have developed probabilistic systems approaches have joined the Probabilistic Systems Assessment Group (PSAG; also known by their former acronym, PSAC, for Probabilistic Systems Assessment Code User's Group), sponsored by the NEA of the OECD. The PSAG has established a set of exercises to compare results and to test various aspects of probabilistic systems assessment codes systems.

The exercises completed to 1990 are known as the PSAC Levels 0, E and 1a Intercomparisons:

- The Level 0 Intercomparison (PSAC 1987) was designed to test the executive code (that portion of the program that invokes the models and usually performs auxiliary functions, such as data input and output and sampling of probability density functions), and the sensitivity analysis used to analyze the results. A set of simple submodels and associated data were used to simulate the processes of waste form leaching, transport of radionuclides through a buffer layer in a vault and through a single layer of rock in a geosphere, and to estimate dose to man from drinking water from a well at the surface of the geosphere. Seven fission products were studied.

- The Level E Intercomparison (PSAC 1989) was also designed to test the executive code. In addition, an analytical solution to the exercise was available for a more comprehensive comparison. This exercise also used simple models representing container failure and transport of radionuclides through two layers of geological media with different hydrogeological properties. Radiation doses result from radionuclides that enter a stream used for drinking water. Four radionuclides were studied: ^{129}I, and the decay chain ^{237}Np, ^{233}U and ^{229}Th.

- The Level 1a Intercomparison had two aims (PSAC 1990). The first was to select and develop appropriate models to describe a hypothetical disposal concept. The second was to apply these models in an assessment code, and then compare the results from the different codes. Thus this exercise provided for some degree of testing of the modelling capability of the participants. The supplied description of the concept included processes such as container failure, waste form leaching and sorption on the media in the vault and geosphere through which radionuclides must travel.

Each of these studies involve comparisons of many different estimated variables. Each study also shows that results using SYVAC3 are in good agreement with the corresponding results from the other groups (PSAC 1987, 1989, 1990). Results from SYVAC also show good agreement with the analytical solution of the Level E Intercomparison. For example, Figures 2.5b and 2.6 of the the Level E report (PSAC 1989) show the estimated peak doses estimated by SYVAC are virtually identical to the peak doses from the analytical solution.

One additional exercise, known as the PSAC Level 1b Intercomparison, was completed in 1992 (PSAC 1993). The Level 1b exercise provides a test for a biosphere model whose specifications are quite different from the corresponding specifications in SYVAC3-CC3. We participated in this exercise using the SYVAC3 executive code with a biosphere model that meets the required specifications and that is based on many of the model-building algorithms used in SYVAC3-CC3. Our contributions are in good agreement with results from other participants (PSAC 1993), providing further support for SYVAC3-CC3.

B.4.2.3 Comparisons Between SYVAC2 and SYVAC3

An interim assessment of long-term impact was carried out using an earlier generation of the code, SYVAC2 (Wuschke et al. 1985). SYVAC3-CC3 has evolved from SYVAC2 and includes refinements to the models that represent the physical system and improvements to the computational algorithms. Both codes use the same basic approach to probabilistic systems assessment, and both were developed to assess the concept for disposal of Canada's nuclear fuel waste.

Although they are closely related, the two codes were developed about five years apart, and many of the development personnel were different. Also, the results from SYVAC2 have been extensively scrutinized, and no significant computational errors were discovered. Thus, a comparison between the two codes contributes to the QA of SYVAC3-CC3.

To perform the comparison, it was necessary to select a case study where both SYVAC2 and SYVAC3-CC3 could be applied. Many improvements were included in SYVAC3-CC3, to better represent the systems and processes involved. For example, SYVAC2 used a simple geosphere model to approximate transport in three homogeneous layers, whereas SYVAC3-CC3 uses a more flexible network model that can include the effects of homogeneous layers, fracture zones, and more than one vault sector (see Davison et al. (1994) and Section 5.4 in the main text).

The case study selected was one in which differences between SYVAC2 and SYVAC3-CC3 were expected to be unimportant. For both codes, it was decided that the models would not be modified. In instances where the models were substantially different, adjustments to the data were sometimes possible so that the differences would be minimized. An example where adjustments were made is for the model describing failure of the containers: SYVAC3-CC3 includes failures resulting from initial fabrication defects, crevice corrosion and delayed hydride cracking, whereas the corresponding model in SYVAC2 includes only uniform corrosion. However, the data for both codes could be adjusted, such that the calculated rates of container failures are similar.

The results of the case study showed satisfactory agreement between the two codes. All significant differences in results were examined and are attributed to differences between the models used in SYVAC2 and SYVAC3-CC3 that could not be resolved by adjustments to the data. The results of this exercise add to our confidence that the SYVAC2-SYVAC3 family of codes is self-consistent within the limitations mentioned above.

B.4.2.4 Intercomparisons Involving the SYVAC3-CC3 Vault Model

The vault model in SYVAC3-CC3 includes a complex solution to a set of partial differential equations that describe contaminant transport through the buffer and backfill (Johnson et al. 1994). To test these solutions, a study was carried out by staff of Ontario Hydro, with two main objectives:

- to develop independently a different solution to the same set of equations, and

- to compare results between the Ontario Hydro solution and the SYVAC3-CC3 solution.

A report describing the contract work concludes that both sets of results correspond very closely (Chan and Advani 1991): most differences are very small and are attributed to differences in assumptions used in the two solution algorithms. Further study of the remaining differences is in progress.

Another code comparison involved the vault model in SYVAC3-CC3 and the AREST code developed for the waste management program in the United States. Only a qualitative comparison could be made because the two codes were originally developed to describe different disposal options. One important difference occurs because the vault model in SYVAC3-CC3 simulates contaminant movement by transport in moving groundwater and by diffusion, whereas AREST accounts only for diffusion (Liebetrau et al. 1987a,b; Apted et al. 1987). Despite these differences, the results of the comparison showed that both codes show similar trends. For example, the two codes showed similar behaviour for the radioactive decay and ingrowth of ^{226}Ra, and similar effects when the rates of container corrosion were varied (Engel et al. 1989).

These two code comparisons add to our confidence that the vault model in SYVAC3-CC3 performs as expected and as required.

B.4.2.5 Intercomparisons Involving the SYVAC3-CC3 Geosphere Model

INTRACOIN, the International Nuclide Transport Code Intercomparison Study, is an international cooperation project for comparing models for release and transport of radionuclides in geologic media (INTRACOIN 1984). The study was conducted before SYVAC3-CC3 was completed; however, the geosphere model in SYVAC3-CC3 was later used to perform the simulations specified in test cases 1 and 2 of the level 1 series of the INTRACOIN study.

The level 1 series focussed on the numerical accuracy of the codes. Test cases 1 and 2 involved radionuclide transport through single and multiple layers of media with uniform hydrogeological properties. Results from the SYVAC3-CC3 geosphere model (described by Davison et al. (1994)) are in excellent agreement with other corresponding results (described in INTRACOIN 1984)).

Another test of the geosphere model in SYVAC3-CC3 was based on the results reported by Gureghian and Jansen (1985). These authors describe the results of a simulation describing the transport of radionuclides in a three-member decay chain through a two-layer medium. Simulations of the same system performed using SYVAC3-CC3 showed excellent agreement (Davison et al. 1994).

Finally, a comparison has been made between the geosphere model in SYVAC3-CC3 and MOTIF (the application of MOTIF to the reference disposal system is described by Davison et al. (1994)). The study, which compared the transport of a nonsorbing tracer (in two-dimensional space using MOTIF and a network of one-dimensional segments using SYVAC3-CC3) show satisfactory agreement (Chan et al. 1991).

B.4.2.6 Intercomparisons Involving the SYVAC3-CC3 Biosphere Model

The SYVAC3-CC3 version of the biosphere model has not been directly compared with other biosphere model codes in model intercomparison exercises. However, in developing the SYVAC3-CC3 code we have generated results comparable to those obtained by other researchers using their research codes. We have also recreated the sample calculation reported in Appendix C of the primary reference for the biosphere model (Davis et al. 1993). This reference describes results obtained using BIOTRAC, a computer code which is functionally equivalent to SYVAC3 and the biosphere model from SYVAC3-CC3 (with modifications to mimic contaminant transport out of the geosphere). We are confident that SYVAC3-CC3 and BIOTRAC give results comparable with the research models on which they are based.

Comparisons to other model codes have been made of the research versions of the component submodels of BIOTRAC: aquatic and terrestrial geosphere/biosphere interfaces, contamination of soil from above and below, and transport through surface waters, the atmosphere and the food chain. The main vehicle of model intercomparison has been the BIOMOVS (Biosphere Model Validation Study) program (Haegg and Johansson 1988). The BIOMOVS program is an international cooperative study to test models for the environmental transfer and bioaccumulation of radionuclides and other trace substances. It was initiated by the Swedish National Institute of Radiation Protection, and includes members from Canada, the United States, Japan and twelve European countries. The first phase of BIOMOVS, which spanned five years and was successfully completed in 1990 is now being supplemented by BIOMOVS II (1992). We are continuing in the international effort to test models designed to quantify the transfer and bioaccumulation of radionuclides and other trace substances in the environment.

In BIOMOVS, the participants defined a number of specific test scenarios involving nuclide transport through some part of the biosphere. Each participant modelled the scenarios independently and submitted results to the project secretariat for compilation and analysis. Differences between the estimates produced by the various models were identified and evaluated in terms of the differences in input data, and in model structure and assumptions. The scenario definitions were set up to encourage diversity of opinion on the processes, pathways and compartments that need to be modelled.

Results from BIOTRAC were submitted for four BIOMOVS scenarios: Scenario B2, irrigation with contaminated groundwater (Grogan 1989); Scenario B6a, discharge to a generic terrestrial zone (Jones 1990); Scenario B6b, discharge to two site-specific terrestrial zones (Jones 1990); and Scenario B7, discharge to a river (Zeevaert 1990). Each BIOMOVS scenario deals with pathways that are central in the movement of nuclides from an underground source through the biosphere and includes the geosphere/biosphere interface in both aquatic and terrestrial settings, soil contamination from both subsurface and above ground sources, and transport through surface waters, the atmosphere, and the food chain. The four scenarios also consider a long time frame and treat radionuclides of importance in the waste management context. Taken together, the four scenarios have exercised key components of BIOTRAC.

As a general rule, all participants calculated the same trends in compartment concentrations. For a given scenario, compartment and radionuclide, the estimates of eventual steady-state concentrations from the various models typically ranged over 2 to 5 orders of magnitude. Results from BIOTRAC were never extremely large nor small but lay within the range of values estimated by the other models (Grogan 1989, Jones 1990, Zeevaert 1990). However, our steady-state concentrations tended to be on the high side. This reflects the conservative bias built into BIOTRAC and is a desirable feature in a model designed for long-term assessments. The large spread in the results arises largely from the nature of the BIOMOVS exercise.

The BIOMOVS study has shown that

- there is a common understanding of the processes and pathways of importance in nuclide transport through the biosphere;

- the BIOTRAC code is consistent with those of others worldwide (and because they are functionally equivalent, we extend this conclusion to the biosphere model in SYVAC3-CC3); and

- our estimates of impact are comparable with others worldwide.

In the assessment of the reference disposal system, the situation is better defined than in the BIOMOVS scenarios, and the parameter values are chosen to reflect the restricted range of possible values; thus the uncertainties are likely to be smaller than those found in the BIOMOVS study.

B.4.3 SENSITIVITY ANALYSIS

The models used in SYVAC3-CC3 have been developed from more fundamental research models based on laboratory and field data. The SYVAC3-CC3 models are meant to simulate the evolution of the important variables of the vault, geosphere and biosphere for the reference disposal system, in accordance with detailed model results. The results of the simulations include identification of those parameters in the SYVAC3 models that should be important for the reference disposal system over long periods of time.

The results of the sensitivity analyses of the models and the system as a whole can be studied to see whether they are reasonable. The results described in Chapter 6 in the main text and Appendices D and E have been presented for review to members of the Canadian nuclear fuel waste management program whose responsibilities involved the development of research models and data. Specifically, the reviewers examined all important parameters that had been identified in the sensitivity analysis of the median- value simulation and the probabilistic simulation. They were asked to confirm that the results from SYVAC3-CC3 are consistent with their understanding of and experience with the more fundamental research models and data. The conclusion of this review has verified the results of the sensitivity analyses, supporting our confidence that the SYVAC3 models faithfully represent the important features of the detailed models from which they were derived.

B.4.4 SUMMARY AND CONCLUSIONS

The QA of the models has involved many approaches. This includes extensive code intercomparison, comparisons with observations of natural analogues (discussed by Cramer (1986, 1993) and Goodwin et al. (1989)) and investigation of model behaviour through sensitivity analysis as well as code functional testing, as discussed in Section B.3.3.9.

Each of these studies have supported our confidence in the accuracy and reliability of the models as they are used in the assessment. They also support our belief that this assessment approach can serve as the basis of the long-term environmental impact assessment of an actual disposal system at a site on the Canadian Shield.

B.5 DATA QUALITY ASSURANCE

B.5.1 INTRODUCTION

The SYVAC3 calculations with the CC3 models require data for many thousands of parameters, contributed by dozens of researchers. These data and the corresponding models and model linkages were constructed through the efforts of the three Model Working Groups responsible for the vault, geosphere and biosphere models in the system model. These same Groups were also responsible for documenting the validation support for the data (and models); this documentation is provided in the primary references for the vault model (Johnson et al. 1994), the geosphere model (Davison et al. 1994) and the biosphere model (Davis et al. 1993).

The discussion here is focussed on measures that give credence to the successful implementation of the data in SYVAC3-CC3. It covers the issues of data consistency and data use in SYVAC3-CC3.

- To ensure consistency in the data set as a whole, data contributors were asked to apply the guidelines in Stephens et al. (1989, 1993) when they recommended parameter values for the postclosure assessment. The guidelines describe the hypothetical disposal system and set down the assumptions made about future climate, the nature of the critical group and other information needed to specify precisely the intended meaning of the assessment simulations.

- To ensure that the intended data is actually used in SYVAC3-CC3, an automated procedure was established to track the transfer of all data from the data contributors through to a SYVAC3 input file. The procedure includes some elements of the above issue to help ensure the data set is consistent.

The discussion below outlines the procedure for handling SYVAC3-CC3 data. A computer database is used to store the data, and computer programs are used to transform and transfer the data whenever possible. This automated approach has the advantages of

- avoiding manual methods that tend to be error-prone when dealing with such large amounts of data, and

- allowing for multiple reviews of data (as noted below).

B.5.2 <u>THE MASTER DATABASE</u>

The database for SYVAC3-CC3 data was designed and implemented to meet the following specific requirements:

- store all data used by SYVAC3-CC3 for the postclosure assessment;

- accept data provided on printed or electronic forms, such as the standard form shown in Figure B-3;

- enable different people to contribute data, but control data entry into the database itself;

- ensure that the data for each model is approved by designated reviewers, so that only approved data can be placed in the database;

- provide checks to ensure that the approved data has been correctly entered into the database; and

- automate generation of input files for SYVAC3-CC3 from the database.

Control of the database is achieved through several integral aspects of the data-handling system. Responsibility for data integrity is assigned to a specific individual, known as the Database Manager, who controls data entry. The computer system file protection facilities limit access to the data, so only the Database Manager can modify these files. Before entering data, the Database Manager must obtain all required reviews and approvals.

The master copy of the database, the Master Data File (MDF), consists of a computer library of word processor files. The MDF was set up using the data requirements of the SYVAC3-CC3 code itself. The data handling programs begin by reading the SYVAC3-CC3 "INCLUDE" files to extract the names of all variables used to store data in SYVAC3-CC3 (specifically, all input and output variables are identified).

Figure B-4 shows the flow of data associated with the database. Most of the data handling is automated from the time data are received from the contributors until they are installed in a SYVAC3-CC3 input file.

Data was entered into the MDF by different routes, depending on the preferences of the data contributor to

- Provide data in written tabular form.

- Provide the data on a standard data form (Figure B-3). For this and the previous case, data entry clerks entered the data into temporary files, until the data were confirmed (described below) and could be moved to the MDF.

SYVAC3-CC3 Parameter Characteristics for the CAD Post-Closure Assessment

1. Data Authorization
Data submitted by:____________________ Date:__________
(signature)

PLEASE TYPE. SEE ESAB GUIDELINES FOR DEFINITIONS OF TERMS.

2. Parameter Full Name, Complete Definition and Mathematical Symbol

Full Name:

Complete Definition:

Mathematical Symbol (if any):

3. SI Units

4. Probability Density Function (PDF) for the Parameter

PDF Type:__________

Bounds: None [ ], or
Value bounds [ ], or
Quantile bounds [ ]

Upper bound:__________

Lower bound:__________

Attributes (a,b,c,μ,σ,GM,GSD,α_1,α_2,n,(a_i,b_i,w_i)) as appropriate for type:
(List on back of page or on a separate page if you need more space.)

___=_______ ___=_______ ___=_______ ___=_______ ___=_______

5. Dependence (if any) on Another Parameter via a Correlation Coefficient

Independent [ ], or
Dependent on parameter:____________________
(Full Name)
with Correlation Coefficient (between -1. and +1.):__________

88-Sep-26 Form ESAB-PC-1 (continued on back)

6. Reasons for This Choice of PDF (Please provide justification for the given information, including PDF type, attributes, bounds, the principal sources of uncertainty, underlying assumptions, simplifications and qualifying conditions, and attach a plot of the PDF and data points used. Alternatively, please provide a reference where this information may be found.)

7. SYVAC3-CC3 Information (TO BE COMPLETED BY ESAB)

Short name of the parameter in SYVAC3-CC3:__________

*Long name (up to 32 characters):*__________

Data are compatible with CC3
model constraints. Checked by:____________________ Date:__________
(signature)

Data have been correctly entered into
SYVAC3-CC3 data base. Checked by:____________________ Date:__________
(signature)

88-Sep-26 Form ESAB-PC-1 (continued from other side)

FIGURE B-3: Sample Form Used to Transfer Data to the SYVAC3-CC3 Master Database

The top line of the form identifies the person contributing the data, and the FORTRAN name of the corresponding parameter in SYVAC3-CC3. Box 1 contains the authorization of the data contributor and chairperson of the Model Working Group for the vault, geosphere or biosphere models. Boxes 2 to 6 describe the parameter, its probability density function (PDF), and the reasons for choosing that PDF. Finally, box 7 contains confirmations that staff in the Environmental and Safety Assessment Branch, Whiteshell Laboratories have made further checks of data compatibility with the model and correct entry into the database.

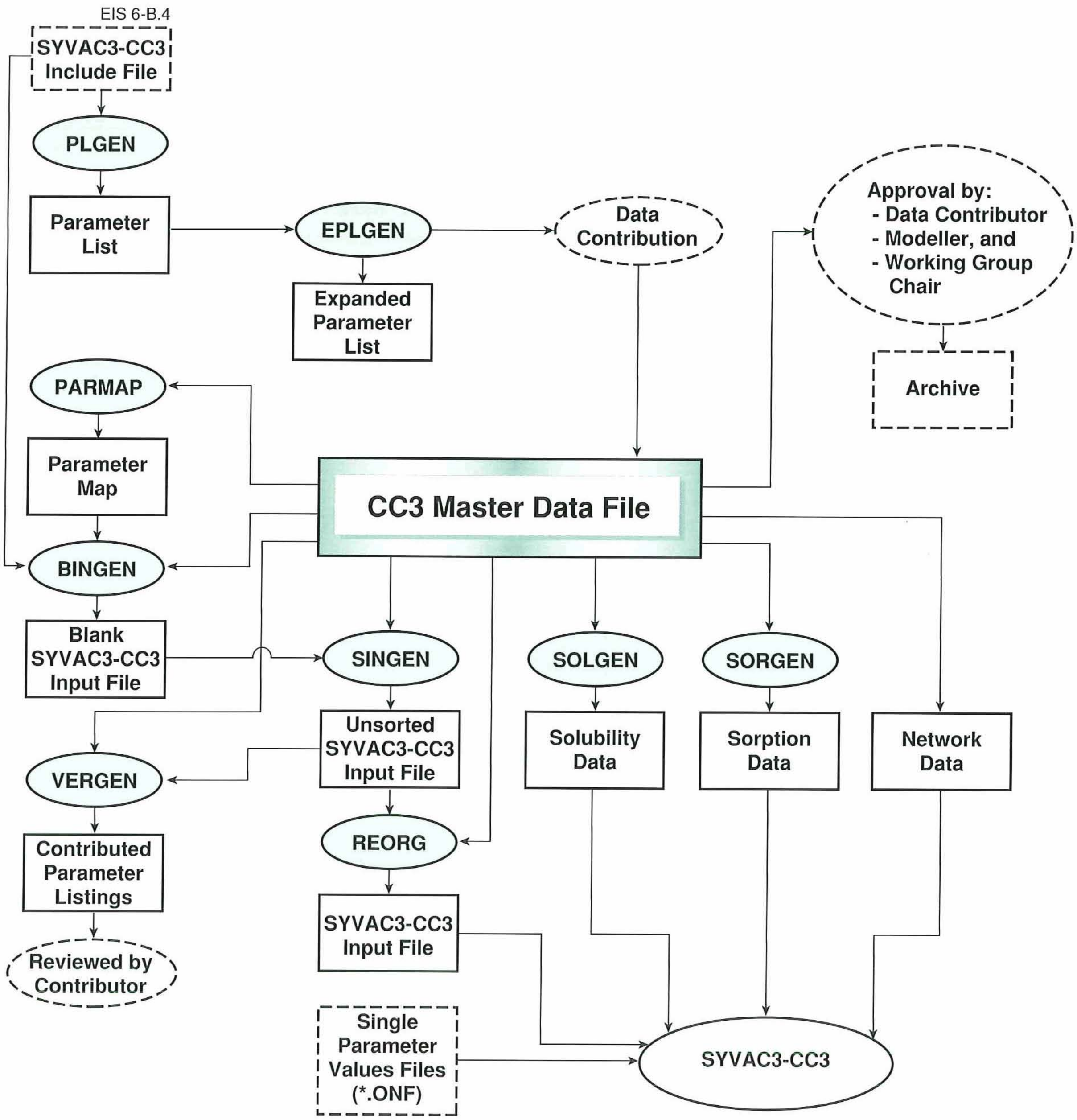

FIGURE B-4: Data Flows Associated with the SYVAC3-CC3 Master Data File

The rectangles designate objects in the system, and the ovals designate processes. The shaded ovals identify computer programs written specifically to handle this data. The dashed outlines indicate items created or processes done manually, at least partially, whereas the solid outlines indicate automation.

- Provide the data on electronic media (such as computer mail). In this instance, the completed files were transferred to the Database Manager, who installed them in temporary files for confirmation and final entry.

For very large arrays of data already stored on computer, special programs were written to arrange the data into the format required for the database. A provisional database was used to recreate the original arrays, which were compared with the contributor's data files to confirm that the data transformations had been done correctly.

For all data entry methods used, printouts of the temporary files were returned for review and confirmation to the data contributor. As well, the printouts were forwarded for review and approval to:

- personnel in the Environmental and Safety Assessment branch responsible for the development of the SYVAC3-CC3 code for the model(s) that use the data; and

- the appropriate chairperson(s) of the vault, geosphere and biosphere model working groups who have overall responsibility for the development of the models and data.

Once all required approvals were available, the Database Manager moved the data from the temporary files into the MDF and archived the original collection of forms containing the formal approval signatures.

Another computer program was developed to extract data from the SYVAC3-CC3 input files. Sample of this data were again verified by the contributors, confirming that no errors had been introduced in producing the MDF or the SYVAC3-CC3 input files.

Changes to data are handled as described above: the new data are entered and held in temporary files until confirmed, and then the existing MDF is updated. Thus the MDF holds only the most recent version of data, although copies of all successive versions are available in archived files.

In a few instances, data for several variations of a given parameter were kept in the data base. For instance, different sets of data were required to describe vault and geosphere properties for a vault with rooms below fracture zone LD1, for another vault with rooms above and below LD1, and for three disposal systems with waste exclusion distances of 30, 50 and 70 m. All the data for these variations were held in files labelled with the name of the case.

B.5.3 CREATING SYVAC3-CC3 INPUT FILES

SYVAC3-CC3 input data files are generated automatically from the master database files, and assessment simulations are performed by a designated individual who has access for creating and modifying these files.

To produce input files for SYVAC3-CC3, a file without numerical values is first created in the format required by SYVAC3-CC3. Parameter names, units and data contributor names are inserted from dictionaries stored in the database, as provided by the system modellers. Then the required parameter distributions are read from the database and inserted into the input file.

In addition to the main input file, SYVAC3-CC3 requires three fixed data files containing solubility data for the vault model, and sorption and segment network data for the geosphere model (Szekely et al. in preparation). Computer codes have been written that generate the first two of these files from data in the database. The third fixed data file does not vary often, and can be reliably generated manually.

Whenever a new version of SYVAC3-CC3 is released, an archive copy of the database, compatible with that version, is also made.

Many data checks are done within SYVAC3-CC3. Input routines ensure that parameter data are correctly stored internally, in variables matching names given in the input file. Where practical, individual modules perform range checks on incoming and outgoing data.

B.5.4 SUMMARY AND CONCLUSIONS

The quality assurance of data has spanned the sequence of steps leading from the laboratory and field research to the assessment code results. Manual handling is minimized, and the data is checked by several experts, each emphasizing a somewhat different perspective.

The procedures and checks provide confidence that the data supplied through the research program are accurately transferred to SYVAC3-CC3 for use in the postclosure assessment.

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APPENDIX C

SAFETY CRITERIA, STANDARDS AND GUIDELINES

CONTENTS

C.1 INTRODUCTION

In Canada, the Atomic Energy Control Board (AECB) is responsible for regulations that apply to the operation of nuclear facilities. The AECB has issued several regulatory documents pertaining to the long-term management of radioactive waste. Three regulatory documents apply to the postclosure assessment: R-71 (AECB 1985), R-104 (1987a) and R-72 (AECB 1987b). Sections C.2 to C.4 discuss aspects of these documents that relate to the postclosure assessment, emphasizing radiological criteria.

Section C.5 describes other considerations that pertain to chemically toxic contaminants and to the protection of the environment.

The federal Environmental Assessment Review Panel (EARP) has issued guidelines (EARP 1992) that provide another source of environmental safety criteria. These criteria have also been taken into consideration for the postclosure assessment.

C.2 THE AECB REGULATORY DOCUMENT R-71

The AECB document R-71, entitled *Deep Geological Disposal of Nuclear Fuel Waste: Background Information and Regulatory Requirements Regarding the Concept Assessment Phase* (AECB 1985), is the primary statement by the AECB that provides the basis for regulatory review and assessment of the concept for disposal of Canada's nuclear fuel waste. It is concerned particularly with the concept assessment stage (if the concept were to be accepted, then R-104 would become the relevant guide for licensing a specific site). The AECB Regulatory Document R-71 defines the following requirements:

- general requirements for a geological disposal system;

- specific requirements for the concept assessment and its documentation; and

- specific requirements for the analysis and predictive modelling of the performance of the disposal system, and its documentation.

The general requirement for the postclosure phase, which begins after closure of the disposal facility, is

> Following closure, the performance of the waste vault must be such that the probability of radiation doses to members of the public, attributable to the existence of the vault, exceeding a small fraction of doses received from natural background radiation will be small. (AECB 1985).

The AECB Regulatory Document R-71 discusses the need to assess the entire disposal system, to perform sensitivity analysis and to have a quality assurance program. It also specifies that the postclosure assessment must include

- estimates of annual effective dose equivalents, and
- evaluation of the significance of inadvertent human intrusion into the vault.

Compliance with the Regulatory Requirements of R-71

The requirements of R-71 are met in the postclosure assessment in discussions of

- the assessment of the entire disposal system, along with descriptions of the behaviour of the vault, geosphere and biosphere subsystems (Chapters 6 and 7 in the main text).
- the results of sensitivity analyses (Chapter 6 in the main text, with details in Appendices D and E).
- quality assurance of models, data and computer codes. This topic is discussed in Appendix B. More details on the models and data are provided in the primary references for the vault model (Johnson et al. 1994a), the geosphere model (Davison et al. 1994a) and the biosphere model (Davis et al. 1993).
- estimates of the annual effective dose equivalent that are attributable to the contaminants placed in the disposal vault (Chapter 6 in the main text).
- inadvertent human intrusion. This topic is discussed in Section 6.8 in the main text for times up to 10^4 a, and is based on a detailed analysis by Wuschke (1991, 1992). The Environmental Impact Statement (EIS) (AECL 1994) provides discussion covering longer time-scales.

C.3 THE AECB REGULATORY DOCUMENT R-72

The AECB Regulatory Document R-72, entitled *Geological Considerations in Siting a Vault for Underground Disposal for High-Level Radioactive Waste* (AECB 1987b) describes the general characteristics of a disposal facility. It discusses several fundamental objectives and requirements:

> ... a successful disposal system for radioactive waste which incorporates both man-made and natural components should
>
> (a) isolate and retain radioactive substances to allow for more complete radioactive decay;
>
> (b) restrict the movement of those radionuclides which may escape from the vault, thus prolonging the time during which further radioactive decay can take place prior to their return to the biosphere; and

(c) restrict human contact with the waste.

Furthermore, in the development of any radioactive waste disposal concept, the following fundamental requirements must be considered:

(a) The disposal system and its components must be capable of accommodating disturbances due to natural phenomena likely to occur in the vicinity of the vault, so that any increase in risk to the public due to the escape of radionuclides as a result of these disturbances would comply with regulatory requirements.

(b) The disposal should be passive; that is, it should be designed to minimize the obligation imposed on future generations to oversee the continued safe isolation of the waste (AECB 1987b).

The AECB Regulatory Document R-72 also describes five geological criteria for an acceptable site:

> The host rock and geological system should have properties such that their combined effect significantly retards the movement or release of radioactive material.
>
> There should be little likelihood that the host rock will be exploited as a natural resource.
>
> The vault site should be located in a region that is geologically stable and likely to remain stable.
>
> Both the host rock and the geological system should be capable of withstanding stresses without significant structural deformation, fracturing or breach of the natural barriers.
>
> The dimensions of the host rock should be such that the vault can be deep underground and well removed from geological discontinuities. (AECB 1987b).

<u>Compliance with the Regulatory Requirements of AECB Regulatory Document R-72</u>

The AECB Regulatory Document R-72 is oriented toward criteria for siting a disposal facility; these criteria are the focus of the primary reference on site screening (Davison et al. 1994b). Nonetheless, some aspects of R-72 are dealt with by the postclosure assessment. In particular, the postclosure assessment provides

- a quantitative description of the ability of natural and man-made barriers to isolate and retain contaminants and to restrict the movement of contaminants that may escape from the disposal vault. The results in Section 6.4 in the main text include detailed discussion of the relative effectiveness of each barrier, considering effectiveness at different times and for different contaminants.

- an overall summary of the effectiveness of the disposal system in restricting human contact with the waste. Results are presented in Chapters 6 and 7 in the main text with additional details in Appendices D and E. The analysis includes consideration of the effects of geological discontinuities, notably the presence of fracture zone LD1, which intersects the horizon of the disposal vault (characteristics of LD1 are described in Sections 5.2 and 5.4 in the main text).

- a discussion of the ability of the disposal system to accommodate disturbances and to be passively safe. These issues are outlined in the discussion of scenario analysis (Chapter 4 in the main text) and in a supporting document (Goodwin et al. 1994). Scenario analysis also deals with the five geological criteria specified in R-72, insofar as they relate to the postclosure assessment. More detailed discussion on these issues is provided in the EIS (AECL 1994), the primary reference on site screening (Davison et al. 1994b), with additional discussion in the primary references for the geosphere model (Davison et al. 1994a), the vault model (Johnson et al. 1994a), the biosphere model (Davis et al. 1993), the engineered barriers (Johnson et al. 1994b) and the conceptual design (Simmons and Baumgartner 1994).

C.4 THE AECB REGULATORY DOCUMENT R-104

The AECB Regulatory Document R-104, entitled *Regulatory Objectives, Requirements and Guidelines for the Disposal of Radioactive Wastes - Long-Term Aspects* (AECB 1987a) presents the quantitative and qualitative regulatory bases for judging the long-term acceptability of options for radioactive waste disposal. It describes three objectives:

> The burden on future generations shall be minimized by: (a) selecting disposal options ... which ... do not rely on long-term institutional controls as a necessary safety feature; (b) implementing these disposal options at an appropriate time ...; and (c) ensuring that there are no predicted future risks to human health and the environment that would not be currently accepted.
>
> Radioactive waste disposal options shall be implemented in a manner such that there are no predicted future impacts on the environment that would not be currently accepted and such that the future use of natural resources is not prevented by either radioactive or nonradioactive contaminants. (AECB 1987a).

The third objective is the protection of human health. This requirement contains a quantitative criterion for the postclosure phase:

> The predicted radiological risk to individuals from a waste disposal facility shall not exceed 10^{-6} fatal cancers and serious genetic effects in a year, calculated without taking advantage of long-term institutional controls as a safety feature. ... risk is defined as the probability that a fatal cancer or serious genetic effect will occur to an individual or his or her descendants. Risk, when defined in this way, is the sum over all significant scenarios of the products of the probability of the scenario, the magnitude of the resultant dose and the probability of the health effect per unit dose.
>
> The level of risk selected ... is a level of risk from other activities that is considered to be insignificant by individuals in their daily lives.
>
> ... a risk of 10^{-6} in a year is the risk associated with a dose of 0.05 mSv in a year. Individual doses of 0.05 mSv in a year are a small fraction ... of the annual dose received by the general population in Canada from natural background radiation... (AECB 1987a).

Figure C-1 illustrates this level of risk by comparing annual doses from several sources of radiation.

The AECB Regulatory Document R-104 also provides guidelines for application of the basic radiological requirements to the postclosure assessment.

Guideline 1: Identifying the Individual of Concern [Section 5.1 of R-104]

> The individual risk requirements in the long term should be applied to a group of people that is assumed to be located at a time and place where the risks are likely to be the greatest, irrespective of national boundaries.
>
> Definition of the lifestyle of the hypothetical group of people should be based on present human behaviour using conservative, yet reasonable, assumptions. The diet and metabolic characteristics of the group should be based on present knowledge, assuming that the basic dietary requirements of future individuals will be the same as those of people alive today.

Guideline 2: Probabilities of Exposure Scenarios [Section 5.2 of R-104]

> The probabilities of exposure scenarios should be assigned numerical values either on the basis of relative frequency of occurrence or through best estimates and engineering judgments.

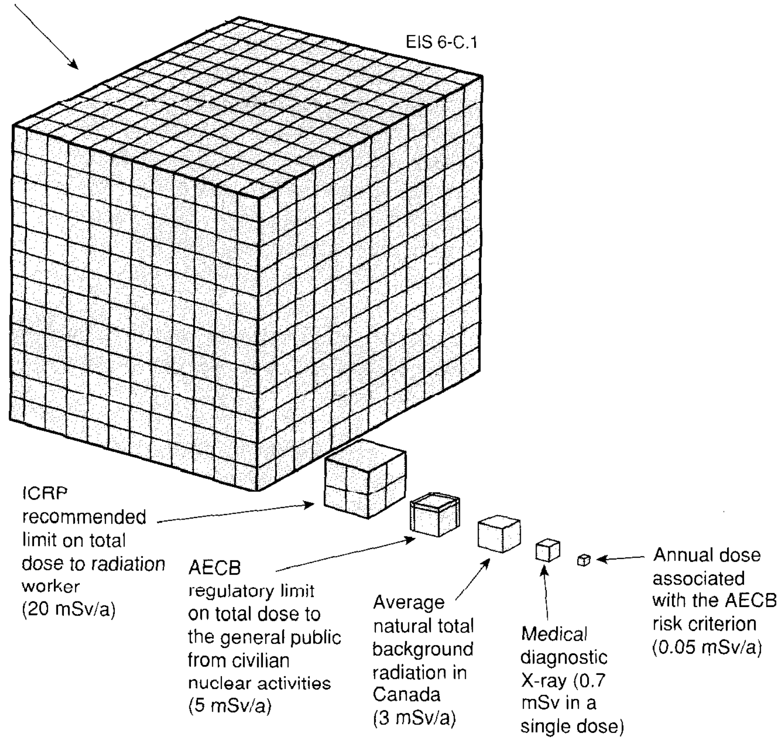

FIGURE C-1: *Comparison of Annual Doses From Different Sources of Ionizing Radiation*

The volumes of the cubes represent the relative magnitude of different radiation doses.

- The largest cube represents a whole-body dose of 5000 mSv in a single exposure, from which there is about a 50% chance of death from radiation sickness. Individuals would be exposed to these severe doses only in the event of a major accident.
- Each small cube in the three largest cubes is approximately equal to the total annual dose from radiation in the natural environment. The third smallest cube illustrates this "natural" annual dose. It amounts to about 3 mSv/a (Neil 1988).
- The second largest cube is the International Commission on Radiological Protection (ICRP 1979) ICRP recommended limit on total annual dose to a radiation worker. The value, 20 mSv/a, is an average over a defined period of 5 a, with a largest permissible dose of 50 mSv in any year.
- The smallest cube represents an annual dose of 0.05 mSv/a. This annual dose is associated with the radiological risk limit established by the Atomic Energy Control Board (AECB 1987a) and is a small fraction (about 2%) of radiation in the natural environment.

The use of subjective probability is appropriate as long as the quantitative values assigned are consistent with the quantitative values of the actual relative frequencies in situations where more information is available. The uncertainty of the probability assigned should also be estimated.

Guideline 3: *Time-scale of Concern* [Section 5.3 of R-104]

The period for demonstrating compliance with the individual risk requirements using predictive mathematical models need not exceed 10 000 a. Where predicted risks do not peak before 10 000 a, there must be reasoned arguments leading to the conclusion that beyond 10 000 a the rate of radionuclide release to the environment will not suddenly and dramatically increase, acute radiological risks will not be encountered by individuals, and major impacts will not be imposed on the biosphere.

Guideline 4: *Output From Predictive Modelling* [Section 5.4 of R-104]

Calculations of individual risks should be made by using the risk conversion factor of 2 x 10^{-2} fatal cancers and serious genetic effects per sievert and the probability of the exposure scenario with either:

(a) the annual individual dose calculated as the output from deterministic pathways analysis; or

(b) the arithmetic mean value of annual individual dose from the distribution of individual doses in a year calculated as the output from probabilistic analysis.

The Environmental Review Panel also cited the need to consider "the potential radiological dose received by humans ... in the vicinity of a site, at critical points in time" (EARP 1992).

Compliance with the Regulatory Requirements of AECB Regulatory Document R-104

Compliance with the requirements and guidelines of R-104 is demonstrated in the postclosure assessment of the reference disposal system. Much of our analysis is focussed on annual dose estimates (ADEs) to members of the critical group. We then use these estimates to calculate the radiological risk.

Risk is calculated using the prescribed equation (AECB 1987a):

$$\text{Risk} = \sum_i p_i \cdot d_i \cdot k \quad . \tag{C.1}$$

Where the summation extends over all significant scenarios,

- p_i is the probability of occurrence of scenario i, as specified in Guideline 2;

- d_i is the annual dose (annual effective dose equivalent) in Sv/a, as specified in R-71, to an individual in the critical group (Guideline 1) and is the estimate for scenario i; and

- k is the risk conversion factor, a constant whose numerical value is 2×10^{-2} fatal cancers and serious genetic effects (or serious health effects) per sievert, as specified in Guideline 4. (Section E.2 in Appendix E notes this risk conversion factor is based on recommendations from ICRP Publication 26 (ICRP 1977). ICRP Publication 60 (ICRP 1991) recommends use of a larger value, 7.3×10^{-2}, for a somewhat different risk end point of fatal and nonfatal cancers or severe hereditary effects. Section E.2 of Appendix E examines the implications of these more recent ICRP recommendations.)

The unit of risk is probability of serious health effects in a lifetime per year of exposure. Figure C-2 illustrates the calculation of risk, assuming that ADEs are known for two hypothetical scenarios.

This definition of risk generally conforms with the definition given by the Canadian Standards Association (CSA) that uses the following equation:

$$\text{Risk} = \text{probability} \times \text{consequence (CSA 1991)}. \qquad (C.2)$$

For radiological impacts, the "consequence" in Equation C.2 corresponds to the product of the annual dose (d_i) and risk conversion factor (k) in Equation C.1.

A modification to Equation C.1 is sometimes recommended for large annual doses; that is, for annual effective dose equivalents that exceed 1 Sv/a. For example, the ICRP (ICRP 1993) and the Nuclear Energy Agency (NEA) (NEA 1984) recommend that it is advisable to assume that a serious health effect will occur if ADEs are greater than 1 Sv/a. This qualification arises because prolonged exposure to large doses is likely to result in serious health effects. The AECB Regulatory Document R-104 does not explicitly qualify Equation C.1. However, an equivalent qualification is implied by Guideline 3, if "acute" radiological risk is taken to apply to situations where there is a high probability of receiving a large annual dose in excess of 1 Sv/a (Section 5.3 of R-104 (AECB 1987a) uses the terms "acute radiological risk" and "acute doses"). We have interpreted Guidelines 3 and 4 in such a manner. Specifically, if scenario j has an estimated mean annual dose that exceeds 1 Sv/a, the product $d_j \cdot k$ is set equal to unity, and the contribution of scenario j to the sum in Equation C.1 is simply its probability of occurrence, p_j multiplied by 1.0 serious health effects per year. It follows that the probability of occurrence of such scenarios must be less than one in a million to meet a radiological risk limit of 10^{-6}.

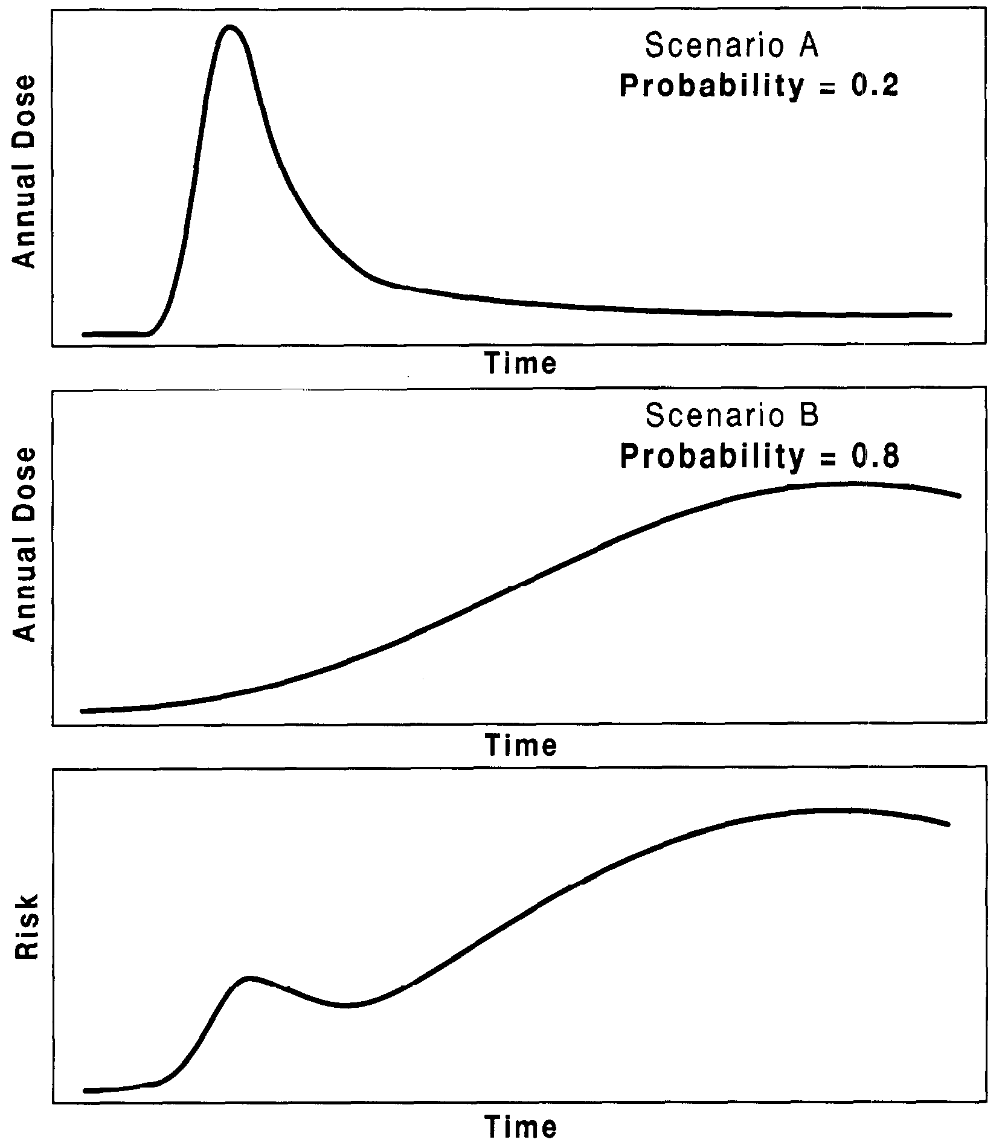

FIGURE C-2: Illustration of an Application of the Risk Equation

The top two curves are for two hypothetical scenarios, showing Annual Dose Estimates (ADEs) plotted against time. In scenario A, the ADE is large at early times and rapidly drops to small values; this might occur, for example, with a relatively mobile and short-lived radionuclide such as ^{14}C. In scenario B, the ADE is small at early times and rises slowly to an intermediate value; this might occur for a less mobile and longer-lived radionuclide such as ^{99}Tc.

Scenario B has a larger (assumed) probability of occurrence (0.8) than scenario A (0.2). These probabilities are used to construct the bottom curve, which shows the risk plotted against time. To construct the risk curve, we first multiply the ADEs from scenarios A and B by their probabilities of occurrence and by the risk conversion factor. We then add these two products, to give the risk curve. The units of risk are probability of a serious health effect per year.

This modification to Equation C.1 leads to larger calculated risk values for ADEs between 1.0 and 50 Sv/a (and smaller values for ADEs greater than 50 Sv/a). In addition, the calculated risk would have a discontinuity if estimated annual doses pass through 1.0 Sv/a: the risk associated with an annual dose equal to 1 Sv/a would be equal to 0.02 p_j, whereas the risk associated with a slightly larger annual dose would be equal to p_j, a value that is 50 times larger.

Guideline 4 implies that calculations of risk can be made using:

- a single ADE, following deterministic pathways analysis. In this case, d_i in Equation C.1 is that ADE for any given year after closure.

- many ADEs, following probabilistic pathways analysis. In this case, d_i in Equation C.1 should be the arithmetic average or mean value of the ADEs for any given year after closure.

Our assessment provides both types of estimates and comparisons in the main text of this report: the former in Section 6.3 and the latter in Section 6.5. However, we consider the probabilistic analysis to be more informative for a decision-making process, because it includes the effects of parameter uncertainty. We show in Section 6.5.1 in the main text that uncertainty has significant effects on the results of the postclosure assessment of the reference disposal system.

We assume that the individual of concern (Guideline 1) is a member of the critical group. Section 5.6 in the main text and the primary reference for the biosphere model (Davis et al. 1993) define the characteristics of the critical group, chosen such that individuals in the group would be exposed to the greatest risk.

Finally, we have addressed Guideline 3 by providing

- quantitative estimates of the annual effective dose equivalents up to 10^4 a following closure. We have actually extended our quantitative estimates to 10^5 a, to demonstrate the performance of the disposal system to the limits of acceptability of the models and data.

- reasoned arguments describing critical aspects of the expected performance of the undisturbed disposal system for long time frames. These arguments are summarized in Chapter 7 in the main text. The EIS (AECL 1994) provides additional discussion on the effects of potential disturbances and disruptions for times beyond 10^4 a.

C.5 OTHER SAFETY CONSIDERATIONS

The AECB documents R-71 and R-104 (AECB 1985, 1987a) and the guidelines from the Panel (EARP 1992) also specify that environmental impacts must be assessed for nonradioactive contaminants released from the disposal facility; however, they do not provide specific criteria, guidelines or standards for nonradioactive contaminants.

In establishing an actual disposal facility, the implementing organization would need to show compliance with all legislation, criteria, guidelines and standards applicable at the time.

For the postclosure assessment of the reference disposal system, we take into consideration the criteria and guidelines noted below. Regulatory requirements are not available for some elements of potential concern (such as technetium and samarium). For these elements, we use very demanding assumed guidelines (such as those discussed in Section 6.5.4 in the main text and by Goodwin and Mehta (1994)) for the comparisons.

The postclosure assessment of the reference disposal system provides estimated concentrations of contaminants in air, water and soil, for comparison with regulatory requirements. We note that two types of calculations are possible, consistent with Guideline 4 for radioactive contaminants (Section C.4). The estimated concentrations may be

- single estimates calculated from deterministic pathways analysis; or

- the arithmetic mean value of estimates from a distribution of estimates calculated using probabilistic pathways analysis.

Our assessment of the reference disposal system includes both types of estimates. However, we consider the probabilistic analysis to be more valuable for decision-making because it includes the effects of parameter uncertainty. Our comparisons with regulatory criteria, therefore, use the arithmetic means of the estimated concentrations.

C.5.1 WATER QUALITY

To protect the quality of water, we examined the most stringent of the following regulations and guidelines.

- *Guidelines for Canadian Drinking Water Quality* (Health and Welfare Canada 1989), issued under the Canada Water Act. This act establishes maximum acceptable concentrations in drinking water for substances known or suspected of causing adverse health effects. The maximum acceptable concentrations are selected to safeguard health on the basis of lifelong consumption and the use of water for all domestic purposes. We also consider guidelines for some additional elements from McNeely et al. (1979).

- *Metal Mining Liquid Effluents Regulations* issued under the Fisheries Act of Canada (Government of Canada 1978). These regulations specify maximum acceptable concentrations of some contaminants in mine effluents.

- *Ontario Water Resources Act* (Government of Ontario 1978). This act provides objectives and regulations for the preservation of the quality and quantity of surface waters and groundwaters in Ontario, so that they are satisfactory for aquatic life, drinking water, agriculture and recreation. It establishes maximum permissible concentrations for metals and other substances in water.

- *Environmental Protection Act* (Government of Ontario 1980). This act specifies regulations for protection of the environment, with general information on parameters to be monitored in industrial effluents.

These sources were used to determine the most demanding regulation or guideline for each chemical element of concern. For elements not covered by a regulation or guideline, we assume concentration limits that we believe have a large margin of safety. The assumed limits use information such as concentrations found in nominally uncontaminated groundwaters of the Canadian Shield, toxicity data for ingestion, and arguments based on chemical analogy (Goodwin and Mehta 1994).

C.5.2 AIR QUALITY

To protect the quality of air, we examined the most stringent limit on contaminant concentrations from *Air Pollution Control Regulations* (Regulation 308) and *Ambient Air Quality Criteria* (Regulation 296) under the Environmental Protection Act of Ontario (Government of Ontario 1980). For elements not covered by a regulation or guideline, we assumed concentration limits that we believe have a large margin of safety. In general, however, our estimated concentrations of contaminants in air are far below concentrations that would likely have any detrimental impact.

C.5.3 SOIL QUALITY

To protect the quality of soil, we examined guidelines for the maximum concentration of metals in soil given in the two Government of Ontario Publications: *Guidelines for the Decommissioning and Cleanup of Sites in Ontario* (Government of Ontario 1989), and *Guidelines for Sewage Sludge Utilization on Agricultural Lands* (Government of Ontario 1986), issued under the Environmental Protection Act of Ontario. These two reports cover only a few elements, and there are no criteria, standards or guidelines that give acceptable levels of concentration in soils for most elements of concern.

We have, therefore, developed another criterion to establish concentration levels that we believe would have no significant chemical toxicity impact. We assume that an acceptable concentration level can be based on the concentration of the element in an "average" soil that is nominally free of contamination. These acceptable levels tend to be extremely small; for example, they are much smaller than any specified guidelines for any element (Goodwin and Mehta 1994). We use these more stringent concentration levels as criteria for soil quality.

C.5.4 PROTECTION OF THE ENVIRONMENT

The criteria, guidelines and standards described above are mostly oriented toward protection of human health. However, it is important that the post-closure assessment also examine what types of impacts might affect the environment in a broader sense. The AECB Regulatory Document R-104 (AECB 1987a) states that

> It is thought likely that the level of radiation protection afforded all human individuals ensures adequate protection of other living species in the environment, although not necessarily individual members of those species. It follows then that by establishing the requirements found in this document [R-104] concerning the radiation health burden on future generations, an appropriate requirement for environmental radiation protection is also formulated.
>
> "However, there is also a need to provide adequate protection for the general environment from the impacts that might arise from either radioactive or nonradioactive contaminants (AECB 1987a).

The Panel has also noted prominently a requirement for protection of the environment (EARP 1992). Their guidelines state

> All discussions of potential long-term environmental impacts should include the corresponding risk figures to natural ecosystems and humans. Potential impacts should be expressed in terms that are readily understandable, such as:
>
> - possible concentrations of radionuclides or other harmful substances at critical reference locations in the rock mass and surface environments;
>
> - the potential radiological dose received by humans and other biota in the vicinity of a site, at critical points in time;
>
> - possible long-term or chronic pollution effects and bioaccumulation in the food chain;
>
> - the potential for additional cancers (EARP 1992).

Although there is a requirement for evaluating impacts on the environment, we have not identified any specific sources that provide well-recognized criteria to judge the acceptability of our results. Therefore, for the postclosure assessment of the reference disposal system, we have followed a methodology that we believe conforms with current thinking and studies on protection of the environment. The methodology, outlined in Section 6.5.4 in the main text, is discussed in more detail by Amiro (1992, 1993) and Davis et al. (1993).

The methodology includes two general steps: identify the contaminants of concern and then evaluate their potential effects. The identification is made by comparing our estimated concentrations of radioactive and non-radioactive contaminants with typical concentrations of the same nuclides that currently exist on the Canadian Shield. We assume that a contaminant from the disposal facility is environmentally acceptable if its addition would not significantly change existing environmental concentrations. That is, our comparison uses environmental increments that are a measure of the variabilities in existing concentrations (Amiro 1992). It should not be assumed that a contaminant is detrimental to the environment if it does not meet this criterion. For the postclosure assessment of the reference disposal system, we apply the criterion to identify contaminants that are of potential concern for protection of the environment, and then we evaluate their potential effects. (For an assessment of an actual disposal facility, the impact of contaminants similarly identified would be evaluated and judged based on available criteria.)

Our evaluation of impacts includes an examination of chemical toxicity effects and radiotoxicity effects. The latter includes evaluation of radiation dose to both human and nonhuman biota. It is generally accepted that protection of all human individuals from radiological effects also protects other species, though not necessarily individual members of those species (ICRP 1977, AECB 1987a). This is because mammals tend to be the most radiosensitive group of organisms (Whicker and Schultz 1982) and humans tend to be long-lived enough for latent effects to appear. In the postclosure assessment, we assume the critical group inhabits the most contaminated parts of the environment and, if the estimated annual dose to the critical group is small, then the annual doses to other species are also likely to be small. Nevertheless, nonhuman organisms could be exposed to larger doses because of their habitat or lifestyle differences, and there could be an effect on certain species without a concomitant effect on humans. For this reason, we also estimate radiation dose to representative nonhuman biota. Comparisons can then be made with the available regulatory criteria or, otherwise, with corresponding environmental baseline data from the Canadian Shield (Davis et al. 1993) to evaluate the expected severity of the impacts to nonhuman biota.

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APPENDIX D

DETAILED ANALYSES OF THE MEDIAN-VALUE SIMULATION

CONTENTS

continued...

CONTENTS (concluded)

D.1 INTRODUCTION

We present in the sections that follow more details of the deterministic analysis, or the analysis of the median-value simulation. In this simulation, all model parameters assume their median values. (The median value is the value corresponding to the 50^{th} quantile of a probability density function (PDF).) We use this analysis to examine and then illustrate important features and processes in the system model, in the absence of obscuring effects arising from random sampling. (Appendix E discusses results of the probabilistic analysis, which is based on random sampling.)

Note that the value of a variable calculated using median values for its parameters is not, in general, identical to the median value of the same variable taken from a set of simulations in which its parameters are randomly sampled. The two values will be different if the variable is calculated using multiplicative or nonlinear combinations of its parameters or if the parameters are described using asymmetric PDFs. Thus for SYVAC3-CC3, the estimated annual dose at any time from the median-value simulation has a different value from the median estimated annual dose at the same time from any set of randomly sampled simulations.

Sections D.2 to D.4 document the detailed analyses of the vault, geosphere and biosphere models when all parameters are fixed at their median values.

Section D.5 presents some information on how the associated sensitivity analyses are conducted for the median-value simulation. Sections D.6 to D.8 then document the results for the vault, geosphere and biosphere models.

Section D.9 provides some of the mathematical background involved with the analysis of barrier effectiveness discussed in Section 6.4.

D.2 RESULTS FROM THE VAULT MODEL

We describe herein the features of the vault model that are observed to most influence the results from the median-value simulation. The vault model is outlined in Section 5.2 and described in more detail by Johnson et al. (1994).

D.2.1 CONTAINER LIFETIME

The first process of interest is container corrosion, leading to failure of the container walls, ingress of groundwater and release of contaminants.

Two failure mechanisms for titanium containers, crevice corrosion and delayed hydride cracking, are temperature dependent. Because estimated temperatures vary within the vault (Figure 3-3), container failure rates also vary with location in the vault. Thus each vault sector has its own distribution of failure rates and failure times.

The highest temperatures occur in the centre of the vault; the lowest, near the edges. Figure D-1 shows the layout of the vault. We will illustrate the temperature-related effects for vault sectors 1, 3 and 11, which encompass the centre and edges of the vault and span the range of temperature-related effects that can occur.

Figures D-2 and D-3 show the fractional rate of failure and the fraction of the containers that have failed as functions of the time for these three sectors. We observe that

- Almost none of the containers fail before 500 a, and almost all fail by 10^4 a after closure.

- The great majority of the containers fail from crevice corrosion.

- Only a few containers fail early because of (assumed) initial fabrication defects. The model for container failure includes the assumption that about one container in every 5000 will fail within 50 a because of defects (Johnson et al. 1994). We have distributed the early failures among the sectors in proportion to the number of containers in each sector. Thus there is a greater likelihood that more defected containers will exist in the larger vault sectors. With the combination of parameters selected for the median-value simulation, between one to five containers fail early in sectors 1 through 6, but no containers fail early in sectors 7 to 12 (because each of sectors 7 to 12 has fewer than 5000 containers.) The failure rate corresponding to the early container failures is too small to be visible in the figures.

- Only a few containers fail because of delayed hydride cracking, starting when an intact container cools to about 30°C. Containers that cool early tend to fail early. They are barely discernible in the plot on the leading edge of the curve, occurring before 1000 a in sectors 1 and 3 and before 2000 a in sector 11. Containers that cool more slowly also fail at a later time because of hydride cracking, but the total number that has already failed is so small (in the median-value simulation) that they are not visible in the figures.

- Peaks occur in the curves as a result of the rising temperature, which increases the rate of crevice corrosion. Multiple peaks occur because of contributions to the rate curves from distinct populations of containers having different local temperatures. This occurs for sector 1 in Figure D-2 but not for sector 11, which is cooler on the average because it has a much smaller areal extent, and a larger proportion of its containers are closer to the edge of the vault.

- Containers in hotter parts of the vault fail earlier than containers in cooler parts of the vault. Thus we observe that the containers in sector 3 tend to fail before those in sectors 1 and 11.

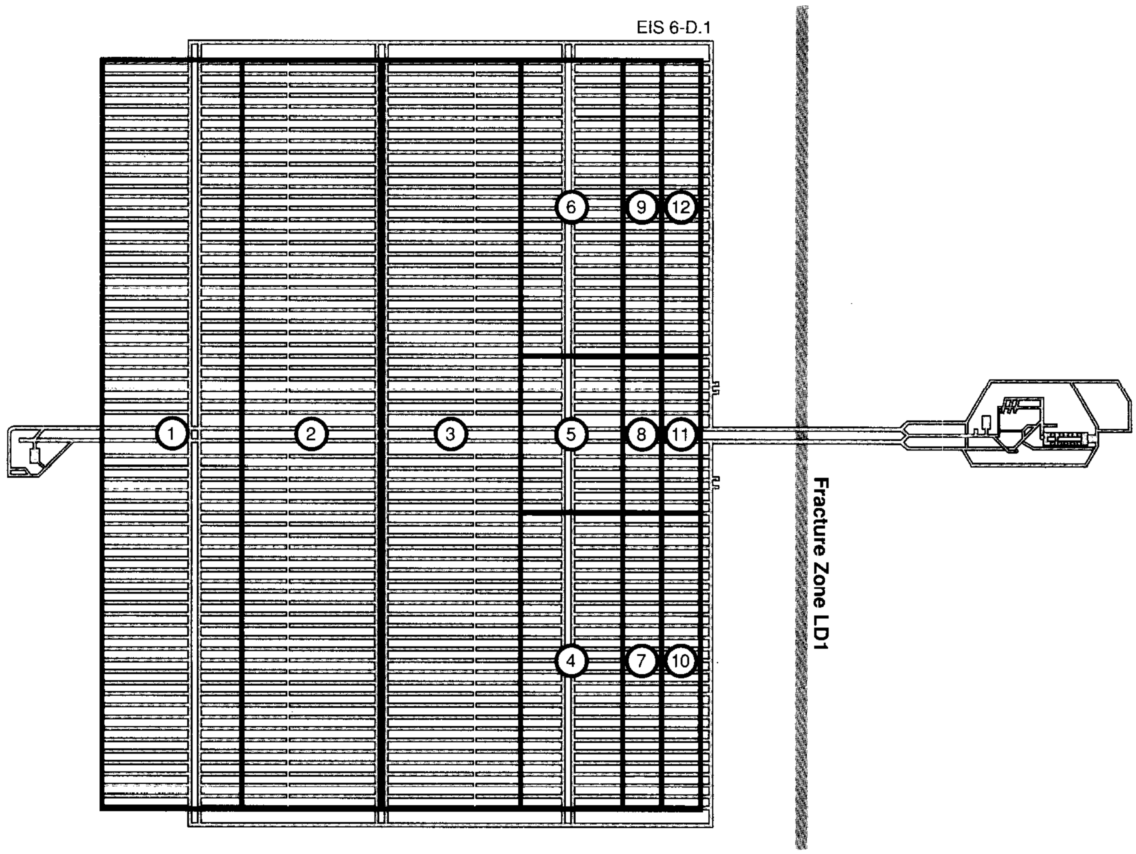

FIGURE D-1: Orientation of the 12 Vault Sectors

Most of the sectors are clustered near fracture zone LD1, where the percentage change in distance to the fracture zone is greatest. Sectors 1 and 11 are at the edge of the vault and are expected to experience cooler temperatures than central sectors such as sector 3.

An examination of data for all sectors shows that sectors 2 through 9 behave much the same as sector 3. For these sectors

- The mode in the container failure rate occurs at about 1900 a; that is, the most probable time of failure of a container is about 1900 a.

- The distribution of failure rates is somewhat skewed such that the average time of failure is slightly greater than the mode.

The mode and average failure times for all containers in the disposal vault would be near the above values because most of the containers in the disposal vault are located in sectors 2 through 9.

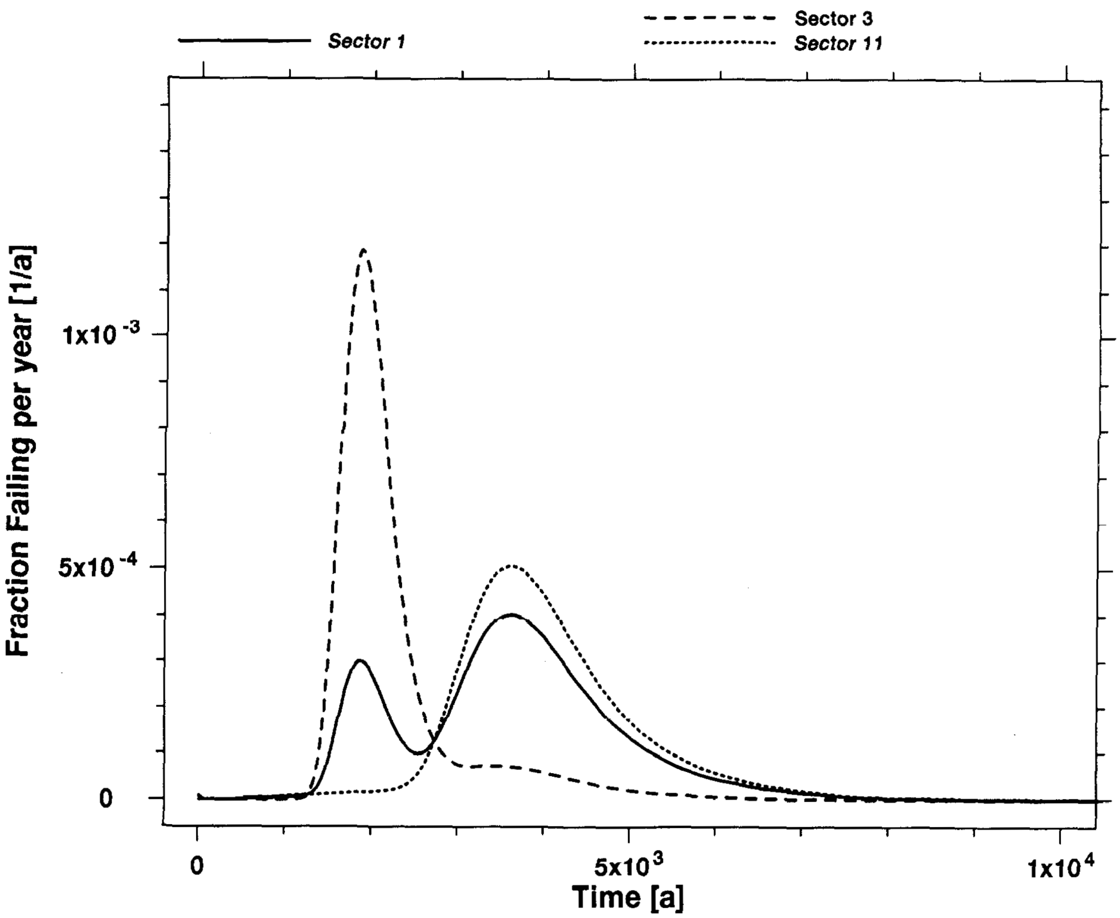

FIGURE D-2: Fractional Rate of Container Failure for the Median-Value Simulation

The fractional rate of failure of the titanium containers is shown as a function of time for sectors 1, 3 and 11. Each curve sums the contributions from the main failure mechanism, crevice corrosion, plus smaller contributions from delayed hydride cracking and initial fabrication defects. Peaks occur because of contributions to the rate curves from distinct populations of containers having different local temperatures. Containers in sector 3 fail earlier because more containers in it experience high temperatures than the containers in sectors 1 and 11.

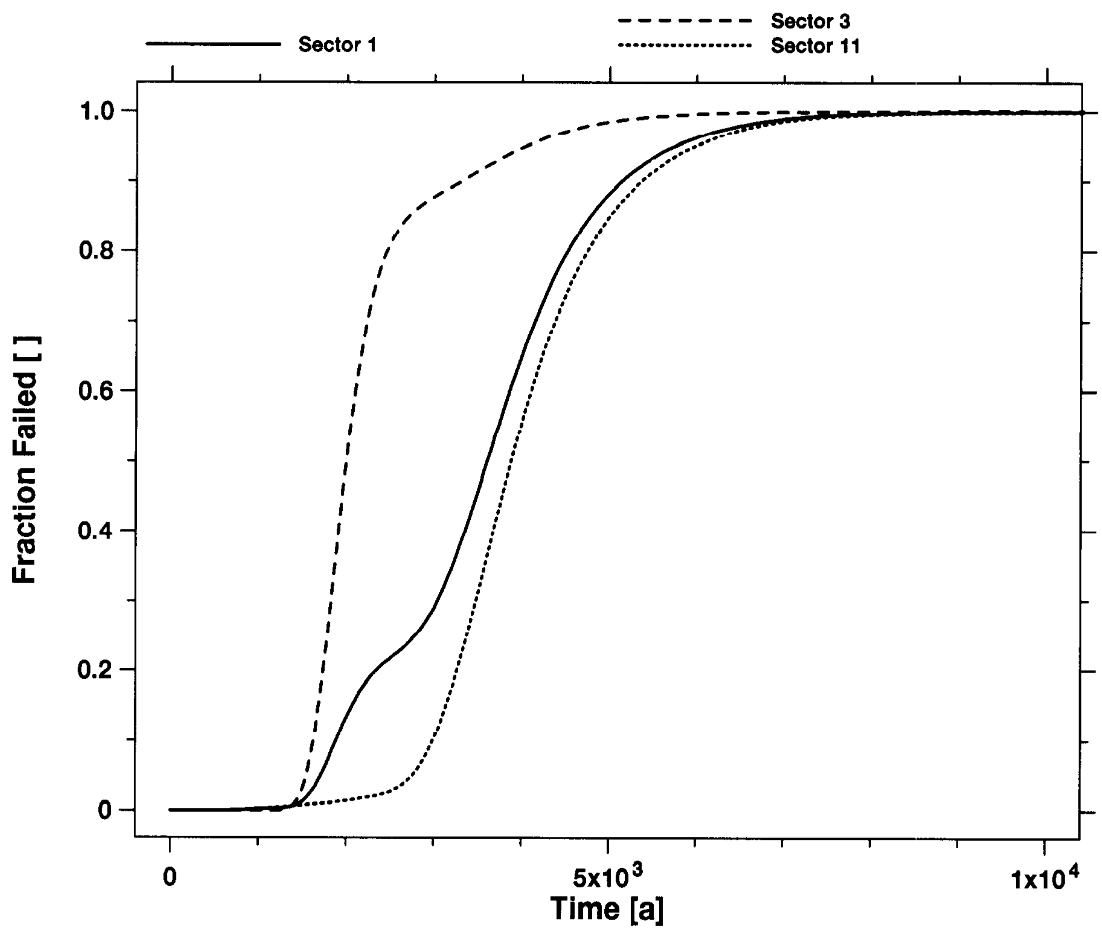

FIGURE D-3: Accumulated Fraction of Containers Failing for the Median-Value Simulation.

These curves show the accumulated fraction of failed containers as a function of time for sectors 1, 3 and 11. They are calculated by integrating the curves in Figure D-2 over time.

Because virtually all the containers fail by 10^4 a after closure in the system model, the entire inventory of contaminants available for instant release is discharged by that time to the container interiors, and then diffuses through the container and through the barriers. At the same time, congruent dissolution of the waste matrices would also be taking place in the failed containers, but (as discussed below) it releases contaminants at a much slower rate.

D.2.2 RELEASE OF CONTAMINANTS FROM THE WASTE MATRICES IN THE VAULT

The two waste matrices in the vault are used fuel and Zircaloy. Contaminants leave the used-fuel waste matrix by both the instant- and congruent-release mechanisms, and the Zircaloy waste matrix by only the congruent-release mechanism (Johnson et al. 1994).

Iodine-129, ^{14}C and ^{99}Tc have different instant-release inventories. For the median-value simulation, these inventories amount to 8.1%, 13.0% and 6.0% respectively of the total ^{129}I, ^{14}C and ^{99}Tc vault inventories. That is, these percentages of the total inventory are released instantly to the container interior upon failure. Because essentially all the containers have failed by 10^4 a after closure, all of the instant-release inventory is available by this time for subsequent transport through the barriers and toward the biosphere. (Recent data for ^{14}C, discussed in the vault model (Johnson et al. 1994), indicate that its instant-release inventory is significantly smaller.)

By contrast, congruent releases are much smaller. The release of each congruently released contaminant is proportional to the rate of dissolution of the matrix material. The geochemical conditions in the vault for the median-value simulation are such that the used-fuel matrix solubility is small (1.55 x 10^{-7} mol/m^3). The dissolution of this matrix is so slow that only a small fraction (6.2 x 10^{-9}) of the UO_2 inventory, with its associated contaminants, is dissolved in 10^5 a.

The solubility of the Zircaloy matrix is also small (1.79 x 10^{-6} mol/m^3) in the median-value simulation. Dissolution of this matrix releases a comparably minute fraction of the zirconium and associated contaminant inventories in 10^5 a.

Figure D-4 illustrates the amounts of ^{14}C released from used fuel and Zircaloy as a function of time. The figure shows that 10^5 a after closure

- Virtually the entire instant-release inventory of ^{14}C (allowing for losses due to radioactive decay) has escaped from the used-fuel matrix.

- Only a tiny fraction of the inventory of ^{14}C available for congruent release has escaped from the used fuel and Zircaloy matrices.

Similar plots for other instant-release contaminants, such as ^{129}I and ^{99}Tc, show equivalent results: most of the instant-release inventory has escaped and most of the congruent-release inventory remains in the waste matrices.

The net effect of these large differences in release is that instant release completely dominates the flow of contaminants to the biosphere and the resulting impacts, for at least 10^5 a after vault closure. As a consequence, we observe that the major contributors to dose are the instantly released radionuclides, notably ^{129}I and ^{14}C from used fuel.

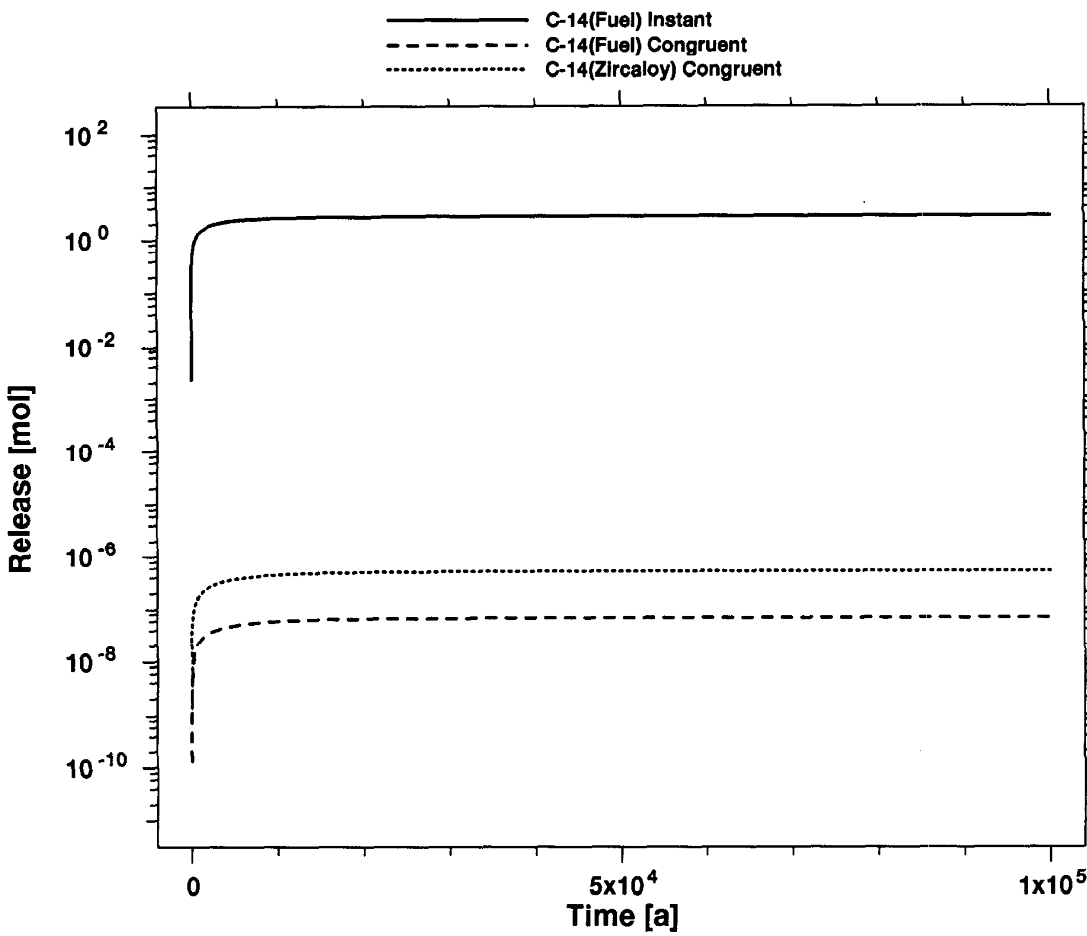

FIGURE D-4: Release of ^{14}C from the Waste Matrices in the Median-Value Simulation

The three curves show the amounts of ^{14}C released as a result of the instant and congruent mechanisms from used fuel, and as a result of the congruent mechanism for Zircaloy. The instant-release mechanism is clearly most important. Note that the vertical axis is logarithmic, to cover the large range of values.

The releases from the used-fuel waste matrix, container, buffer and backfill are illustrated in the set of curves in Figure D-5 for ^{129}I and in Figure D-6 for ^{14}C, for the first 10^5 a after closure. We have chosen to illustrate the releases from vault sector 11 in this and other figures. As we will see in Section D.4, contaminants from this sector contribute most to radiological impacts.

Curves (a) of these figures show the release rate of ^{129}I and ^{14}C from the used-fuel waste matrix; this is based on the assumption that all the containers in sector 11 have failed at time equal to zero. The curves show that these contaminants begin diffusing immediately in the buffer at steadily declining rates, which fall by about a factor of 10 in the first eight years after container failure. As noted above, the instant-release process dominates the shape of these curves.

Curves (b) of Figures D-5 and D-6 combine the effects of waste-matrix release and container failure. They show the total releases of ^{129}I and ^{14}C into the buffer in vault sector 11 as a function of time. These total releases to the buffer are obtained using a mathematical convolution integral, which combines

- the failure rate of containers in sector 11 as a function of time throughout the 10^5-year time period (this release rate curve is shown in Figure D-2); and

- the waste-matrix release rates, also as a function of time (curves (a) of the two figures).

Curves (b) show the total release rates of ^{129}I and ^{19}C from the containers into the buffer have essentially the same shape as the curve of the fractional rate of container failure. This occurs because the waste-matrix release rates are large for only a few years after failure. The release rates into the buffer peak at a few thousand years after closure, at the time when the container failure rate reaches its maximum.

Curves (c) through (e) of Figures D-5 and D-6 are discussed in the next section.

D.2.3 MOVEMENT OF CONTAMINANTS THROUGH THE BUFFER AND BACKFILL

The movement of groundwater in the buffer and backfill is slow: the groundwater velocity in the backfill is about 10^{-6} m/a and even lower in the buffer. Consequently, diffusion is the dominant mechanism of contaminant transport in both barriers.

The rate of transport by diffusion of contaminants in the buffer and backfill is controlled largely by the diffusion coefficients and the barrier capacity factors:

- The diffusion coefficients describe the rate of movement of contaminants by diffusion. Smaller diffusion coefficients correspond to slower transport of contaminants through the medium.

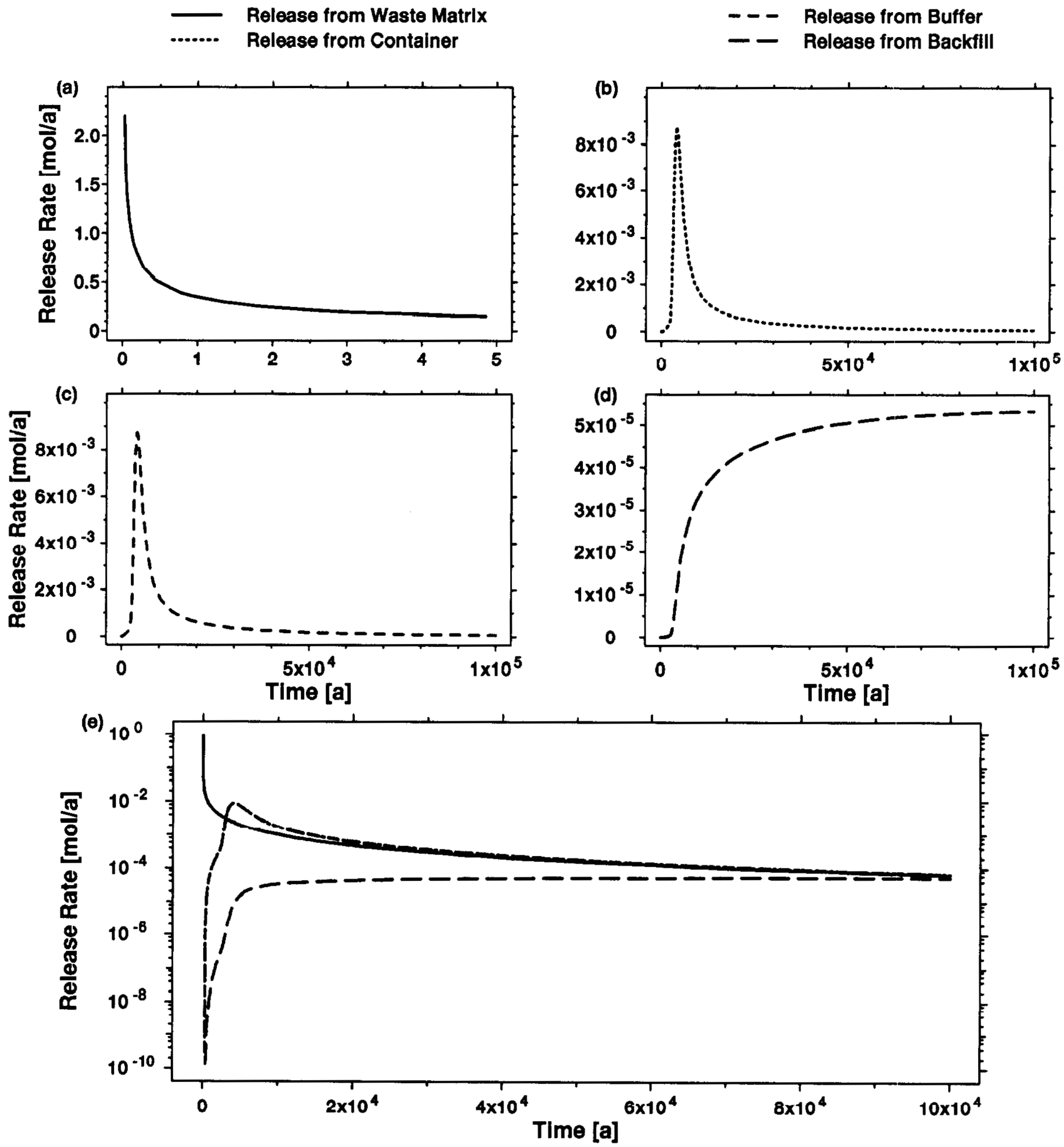

FIGURE D-5: Release Rates of ^{129}I From Sector 11

Each plot shows release rates for ^{129}I versus time (note the different axes scales). The first four plots show, as a function of time, the rate of release of ^{129}I from:

(a) the used-fuel matrix (we assume that all containers in the sector have failed at time equal to zero),

(b) the containers,

(c) the vault buffer, and

(d) the vault backfill to the rock surrounding sector 11.

The plot labelled (e) shows the same data in plots (a) through (d), except that it uses a logarithmic scale for the vertical axis. The plots show that the backfill is particularly effective in delaying and attenuating the movement of ^{129}I.

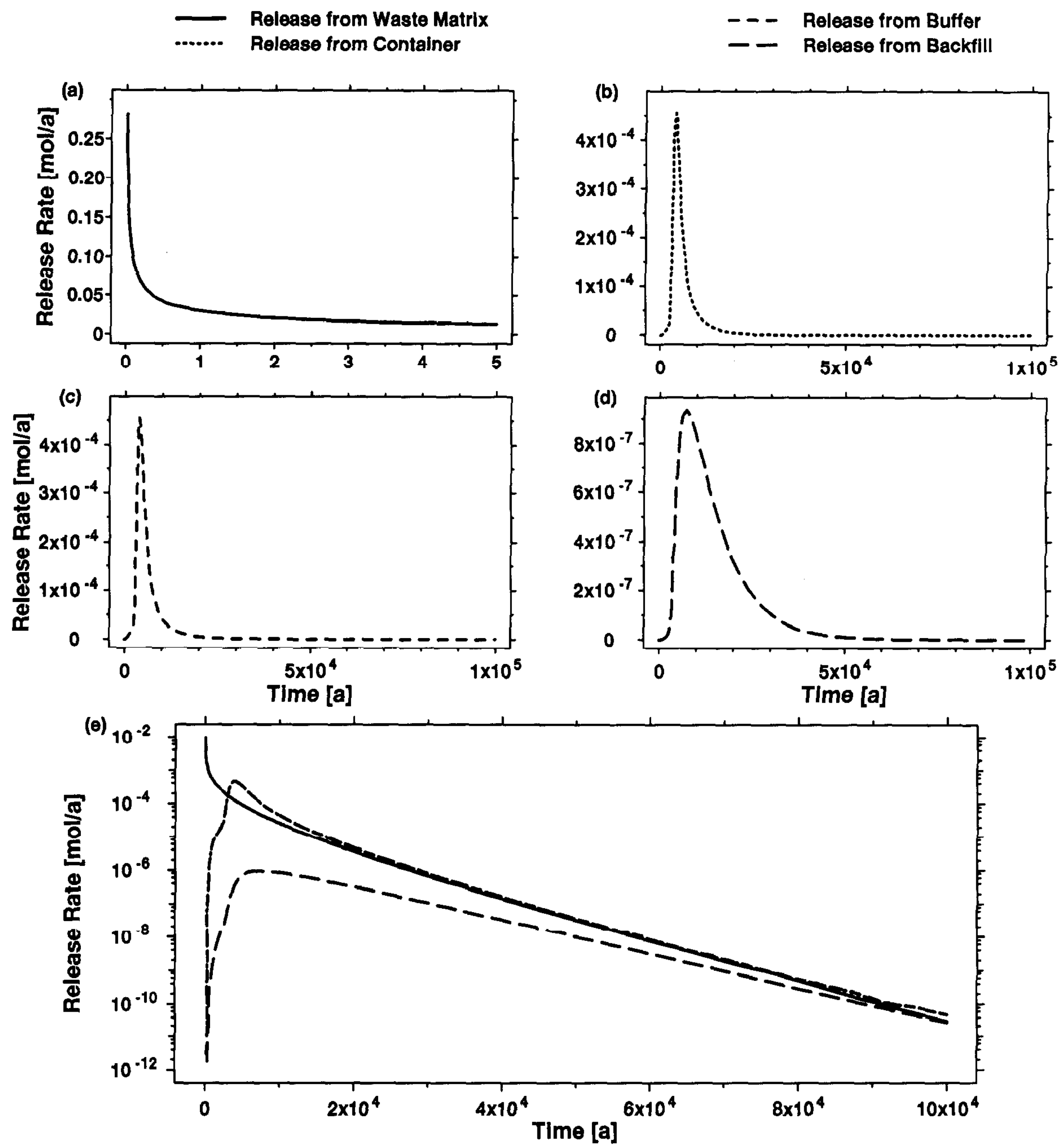

FIGURE D-6: Release Rates of ^{14}C From Sector 11

Each plot shows release rates for ^{14}C versus time (note the different axes scales). The first four plots show, as a function of time, the rate of release of ^{14}C from

- (a) the used-fuel matrix (we assume that all containers in the sector have failed at time equal to zero),
- (b) the containers,
- (c) the vault buffer, and
- (d) the vault backfill to the rock surrounding sector 11.

The plot labelled (e) shows the same data in plots (a) through (d), except that it uses a logarithmic scale for the vertical axis. The plots show that the backfill is particularly effective in delaying and attenuating the movement of ^{14}C.

- The capacity factor is defined as the ratio of the total concentration of contaminant in the medium to the concentration in the water permeating it (Eriksen, 1989). It includes the effects of contaminant sorption and the effects of porosity of the medium. Larger capacity factors delay transport because the medium has a greater capability to store contaminants.

Iodine-129 and ^{14}C are not sorbed in the buffer, and their capacity factors are numerically equal to the porosity of the medium. The porosity of the medium is dependent on the chemistry of the contaminants. Both ^{129}I and ^{14}C are expected to exist as anionic species in groundwater (Johnson et al. 1994), and they would be restricted to the spaces between the clay particles making up the buffer (Cheung and Gray 1989). These interparticle spaces comprise only a small fraction (0.0063 in the median-value simulation) of the volume of the clay medium. Thus the capacity factors for ^{129}I and ^{14}C are small, and these contaminants pass through the buffer with little delay. However, the small porosity of the buffer restricts the total amounts that can pass through the medium at any particular time.

Curves (c) of Figures D-5 and D-6 show the release rates of ^{129}I and ^{14}C from the buffer to the backfill. Because there is no significant delay of these contaminants in the buffer, the release curve from the buffer is approximately the same as the release curve from the containers (compare curves (b) and (c)).

Curves (d) illustrate the release rates of ^{129}I and ^{14}C from the backfill to the rock surrounding sector 11. It is clear that the backfill is effective in delaying their transport. For example, the maximum release rate occurs at 10^5 a after vault closure for ^{129}I. (This time of maximum equals the end of the time period simulated in the median-value simulation. If the simulations were carried to longer times, a global maximum would occur after about 10^6 a.) The delay offered by the backfill, combined with dispersion in this barrier, also attenuates the magnitude of ^{129}I release rates compared with its release rates from the buffer.

Several factors contribute to the long delay of ^{129}I and ^{19}C in the backfill. In the case of iodine

- The backfill has a larger porosity than the buffer (0.25 versus 0.0063 for anionic contaminants) because it has a smaller clay content and, also, is less compacted.

- The larger porosity of the backfill acts as a sink, drawing iodine out of the buffer. Once in the backfill, the iodine leaks slowly into the rock because of the smaller porosity (3.0×10^{-3}) of the sparsely fractured rock surrounding the vault; and

- There is a much larger thickness of backfill to traverse than buffer (1.4 m versus 0.25 m; see Figure 5-9).

Similar comments apply to ^{14}C, except that radioactive decay strongly influences the release rate of ^{14}C. Carbon-14 has a relatively short half-life compared with ^{129}I (5.73×10^3 a versus 1.57×10^7 a). Thus the release rates from the waste matrix, containers, buffer and backfill drop more quickly for ^{14}C than for ^{129}I after the first 10^4 a. This effect is more obvious on a logarithmic scale: compare curves (e) of Figures D-5 and D-6. The maximum release of ^{14}C from the backfill occurs at about 10^4 a (curve (d) of Figure D-6); beyond this time, ^{14}C releases are strongly reduced by radioactive decay. As was the case for ^{129}I, the delay of ^{14}C in the backfill results in a reduction of the backfill release rate and a shift of the peak backfill release rate so as to be later than the peak buffer release rate.

As noted previously, the backfill is so effective in delaying and attenuating the flow of contaminants that, at 10^5 a, the estimated release rate of ^{129}I from the backfill has not yet reached a global maximum. Similar or larger delays and attenuation are observed for all other contaminants, particularly for those that sorb onto the buffer and backfill.

D.2.4 TECHNETIUM-99 RELEASE AND PRECIPITATION IN THE VAULT

The vault model takes into account the possibility of precipitation of contaminants in the buffer. This process is especially important for ^{99}Tc. (Both ^{129}I and ^{14}C are relatively soluble, and their precipitation does not occur in the median-value simulation.) Another important process for ^{99}Tc is its strong sorption onto the buffer and backfill.

Figure D-7 shows the release curves for ^{99}Tc for vault sector 11:

- Curve (a) shows the release rate of ^{99}Tc from the used-fuel waste matrix; this is based on the assumption that all the containers have failed at time equal to zero. Instantly released ^{99}Tc also dominates the total releases of ^{99}Tc.

  The buffer has a large capacity factor for ^{99}Tc (52.8 for ^{99}Tc versus 0.0063 for ^{14}C and ^{129}I). This is largely the result of sorption and moves ^{99}Tc relatively quickly out of the waste matrix. Consequently, the waste-matrix release rate is initially large but drops more quickly for ^{99}Tc than for ^{129}I (curves (a)). Almost all the instant inventory of ^{99}Tc has been released from the containers by 10^5 a, compared with only about 20% of the instant inventory of ^{129}I.

- Curve (b) shows the release rate of ^{99}Tc from the waste matrix and failed containers to the buffer. It is obtained by taking into account the effect of container failure on curve (a).

- Curve (c) shows the estimated release of ^{99}Tc from its precipitate within the buffer. This curve is similar to curve (b), with an attenuated release rate at short times and a slightly elevated rate at longer times. This effect is due to the precipitation of ^{99}Tc (Johnson et al. 1994); the solubility of ^{99}Tc in the buffer is 2.87×10^{-6} mol/m^3 in the median-value simulation. The curve shows a peak that is due to the effect of the rate of failure of the containers. The remainder of the curve is determined by the rate of dissolution of the precipitate.

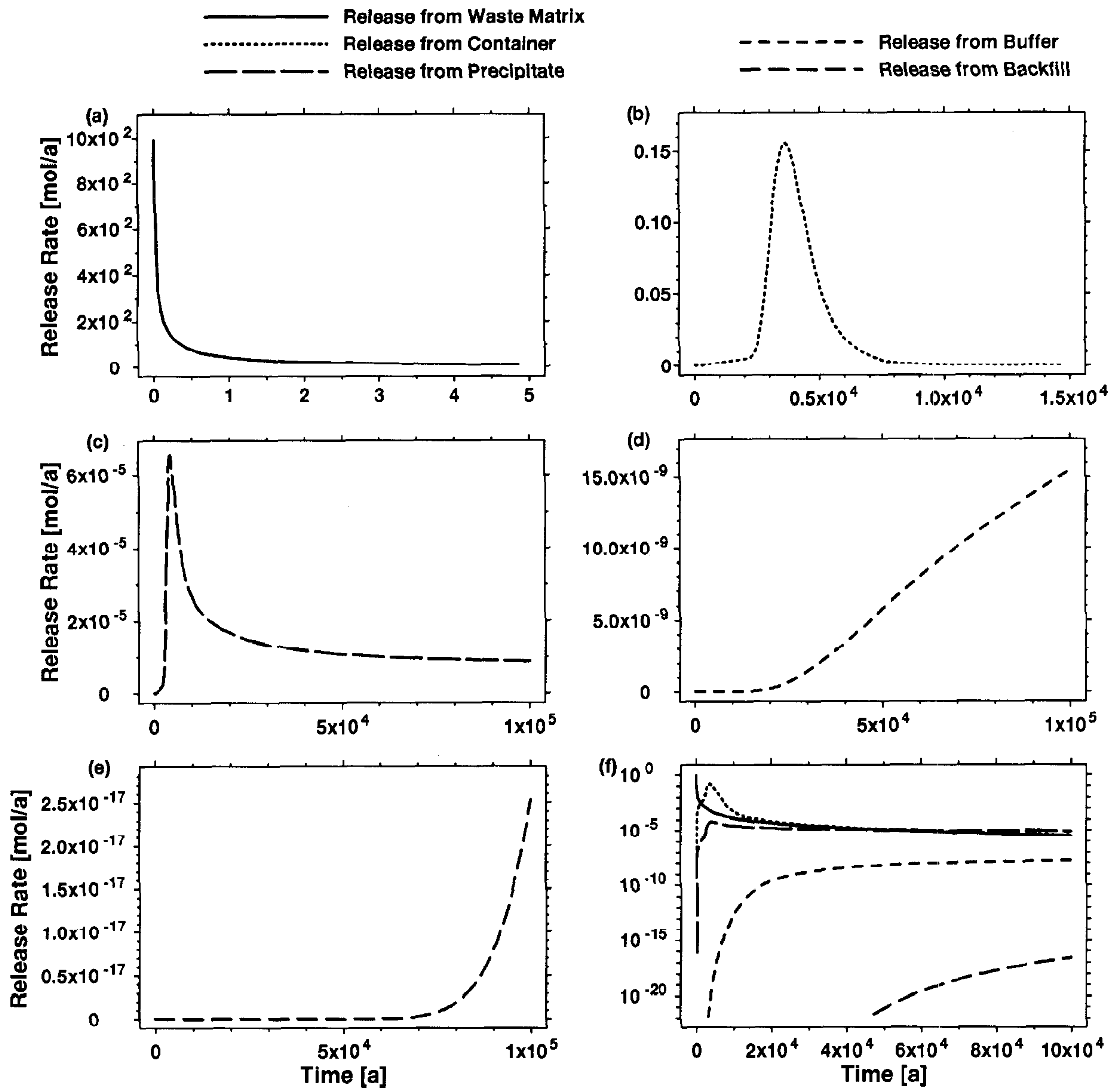

FIGURE D-7: Release Rates of ^{99}Tc From Sector 11

Each plot shows release rates for ^{99}Tc versus time (note the different axes scales). The first five plots show, as a function of time, the rate of release of ^{99}Tc from

(a) the used-fuel waste matrix (we assume that all containers in the sector have failed at time equal to zero),
(b) the containers,
(c) its precipitate within the vault buffer,
(d) the vault buffer, and
(e) the vault backfill to the rock surrounding sector 11.

The plot labelled (f) shows the same data in plots (a) through (e), except that it uses a logarithmic scale for the vertical axis. The plots show that precipitation and the buffer and backfill are particularly effective in delaying and attenuating the movement of ^{99}Tc.

An integration of the precipitate release rate (curve (c)) shows that the total amount of ^{99}Tc released by re-dissolution of the precipitate is about 1000 times smaller than the total release from the waste matrix and containers (curve (b)) for 10^5 a after closure. Thus precipitation in the buffer is an important mechanism in reducing the release of ^{99}Tc (and other sparingly soluble nuclides).

- The precipitate release rate is then convolved with the buffer transport response function, which accounts for a significant degree of sorption of ^{99}Tc in the buffer. This convolution, therefore, produces a much delayed and attenuated release rate from the buffer, shown in curve (d).

- Curve (e) shows that strong sorption of ^{99}Tc in the backfill results in further delay and reduction in its release from the backfill.

These effects are more obvious in curve (f) of Figure D-7, which uses logarithmic scales on the vertical axis.

D.2.5 THE ^{238}U DECAY CHAIN

Uranium-238 is a member of the 4n+2 decay chain, and the vault model simulates the transport of six radionuclides from this chain. Plutonium-242 and ^{238}Pu are treated separately, and four radionuclides are modelled using the simplified decay scheme (Goodwin and Mehta 1994):

$$^{238}U \longrightarrow {}^{234}U \longrightarrow {}^{230}Th \longrightarrow {}^{226}Ra.$$

The transport of other members of the original chain are not simulated in the vault model. Their concentrations within vault can be calculated assuming secular equilibrium: ^{234}Th is in secular equilibrium with ^{238}U, whereas ^{222}Rn, ^{210}Pb, ^{210}Bi, ^{210}Po are in secular equilibrium with ^{226}Ra (other short-lived radionuclides, such as ^{218}Po and ^{214}Bi, are considered implicitly through adjustments to the dose conversion factors of their precursors (Goodwin and Mehta 1994)).

Figure D-8 shows the total inventory in the disposal system of ^{238}U, ^{234}U, ^{230}Th and ^{226}Ra as a function of time. The inventories of ^{238}U and ^{234}U are only slightly decreased over 10^5 a because these radionuclides have long half-lives (4.5×10^9 and 2.44×10^5 a respectively). In contrast, the inventories of ^{230}Th and ^{226}Ra show an increase because of ingrowth from their precursors. The inventory of ^{234}U also has a small increase that is due to ingrowth from ^{238}U.

The large inventory of ^{238}U and the long dissolution time of the used fuel suggest that ingrowth of ^{238}U progeny would continue for time-scales much greater than 10^5 a. The resulting long-term dose potential of these radionuclides is discussed in Chapter 7 in the main text.

The release rates of ^{238}U, ^{234}U, ^{230}Th and ^{226}Ra from vault sector 11 are shown in Figures D-9 to D-12 respectively. The curves in each figure show the release rates from the waste matrix (assuming that all containers have failed at time equal to zero), the containers, the buffer and the backfill.

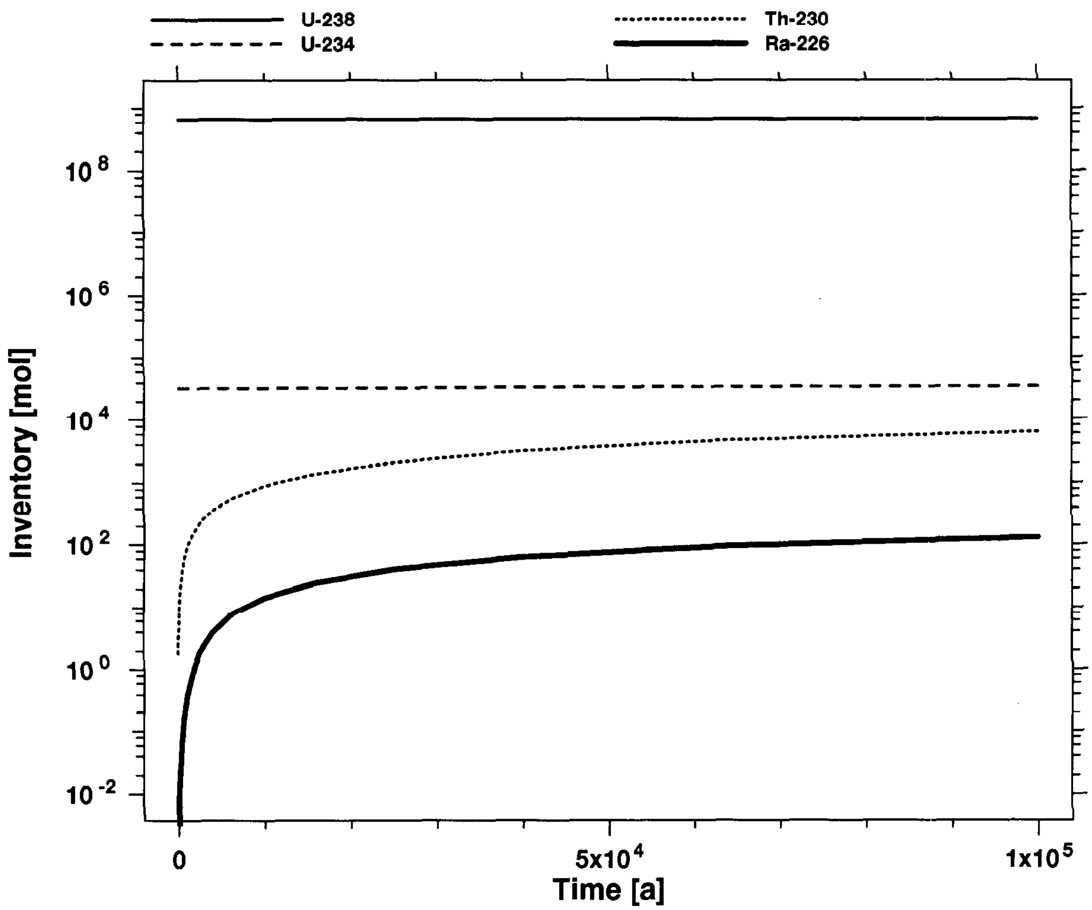

FIGURE D-8: Inventories of Members of the ^{238}U Decay Chain as a Function of Time

The vertical axis uses a logarithmic scale to span many orders of magnitude. These curves show the total inventories of ^{238}U, ^{234}U, ^{230}Th and ^{226}Ra in the disposal system for times up to 10^5 a. Uranium-238 and ^{234}U have long half-lives (4.5×10^{10} and 2.4×10^5 a respectively), and their inventories do not change significantly. The inventories of ^{230}Th and ^{226}Ra show an increase caused by ingrowth from their precursors.

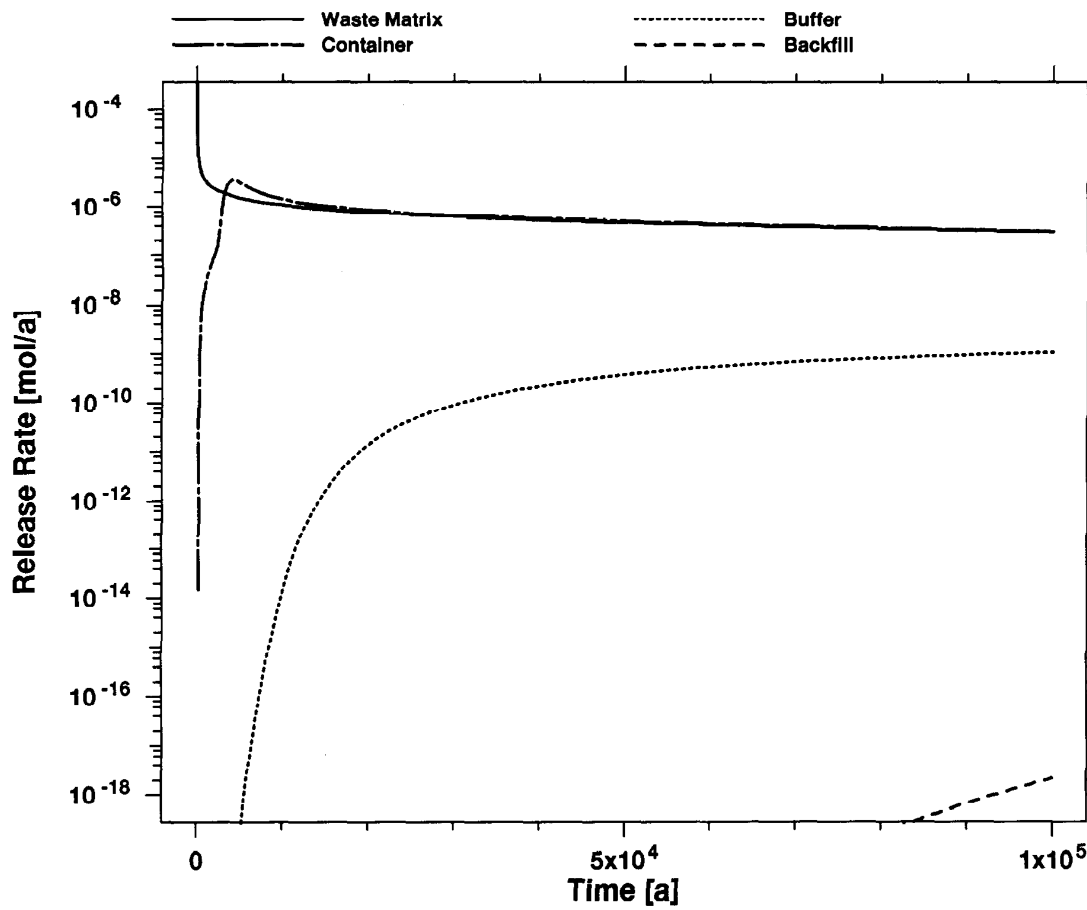

FIGURE D-9: Release Rates of ^{238}U from Sector 11

This figure is similar to previous figures, except that it shows the results for ^{238}U from the used-fuel matrix using a logarithmic vertical scale. The four curves show, as a function of time, the rates of release of ^{238}U from

(a) the used-fuel waste matrix,
(b) the containers,
(c) the vault buffer, and
(d) the vault backfill to the rock surrounding sector 11.

Uranium-238 is the most abundant radionuclide in the used-fuel matrix, but sorption in the buffer and backfill limit its release to insignificant quantities, even after 10^5 a.

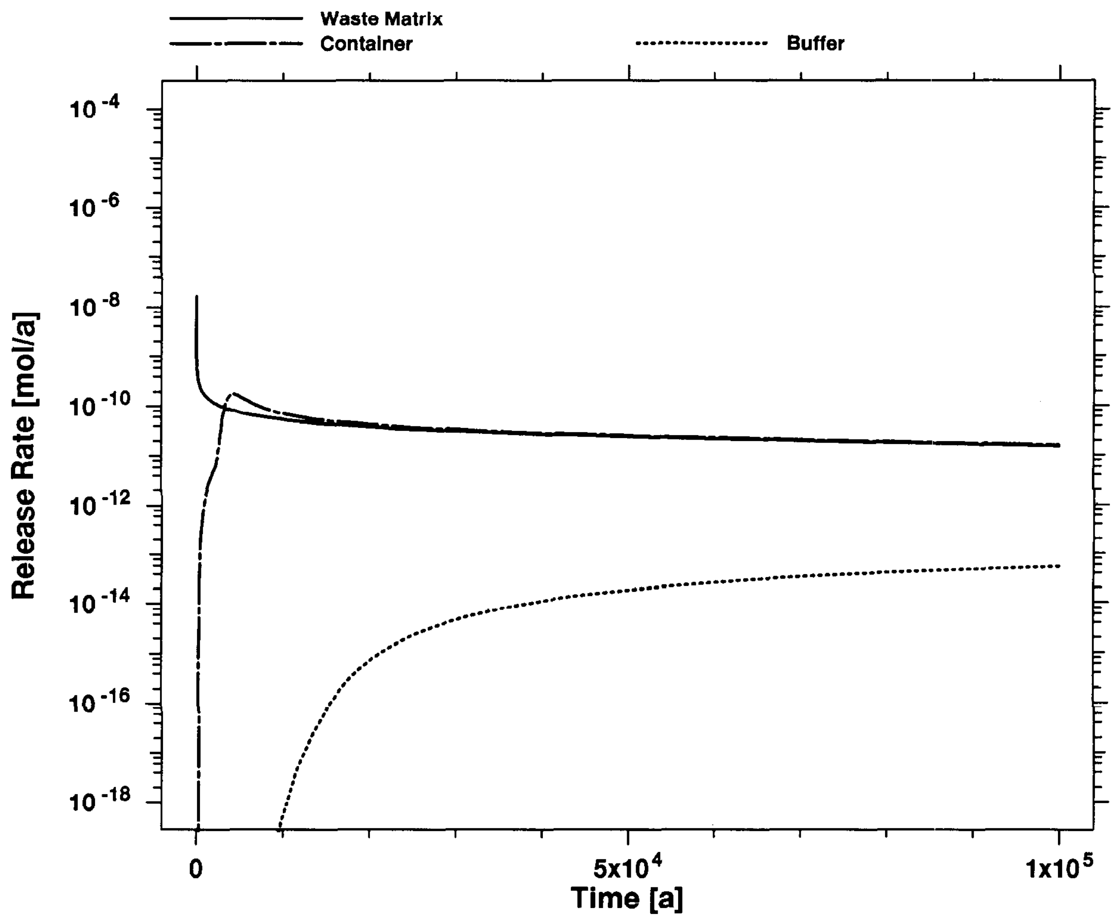

FIGURE D-10: Release Rates of ^{234}U from Sector 11

This figure is similar to previous figures, except that it shows the results for ^{234}U from the used-fuel matrix using a logarithmic vertical scale. The three curves show, as a function of time, the rates of release of ^{234}U from

(a) the used-fuel waste matrix,
(b) the containers, and
(c) the vault buffer.

The rate of release of ^{234}U from the vault backfill to the rock surrounding sector 11 cannot be shown on this plot because the estimated values are less than 10^{-20} mol/a at all times. These curves have a similar shape to those in Figure D-9 for ^{238}U because both radionuclides are isotopes of the same chemical element. The major difference between releases for ^{234}U and ^{238}U is in their magnitudes and can be attributed to the difference in their initial inventories.

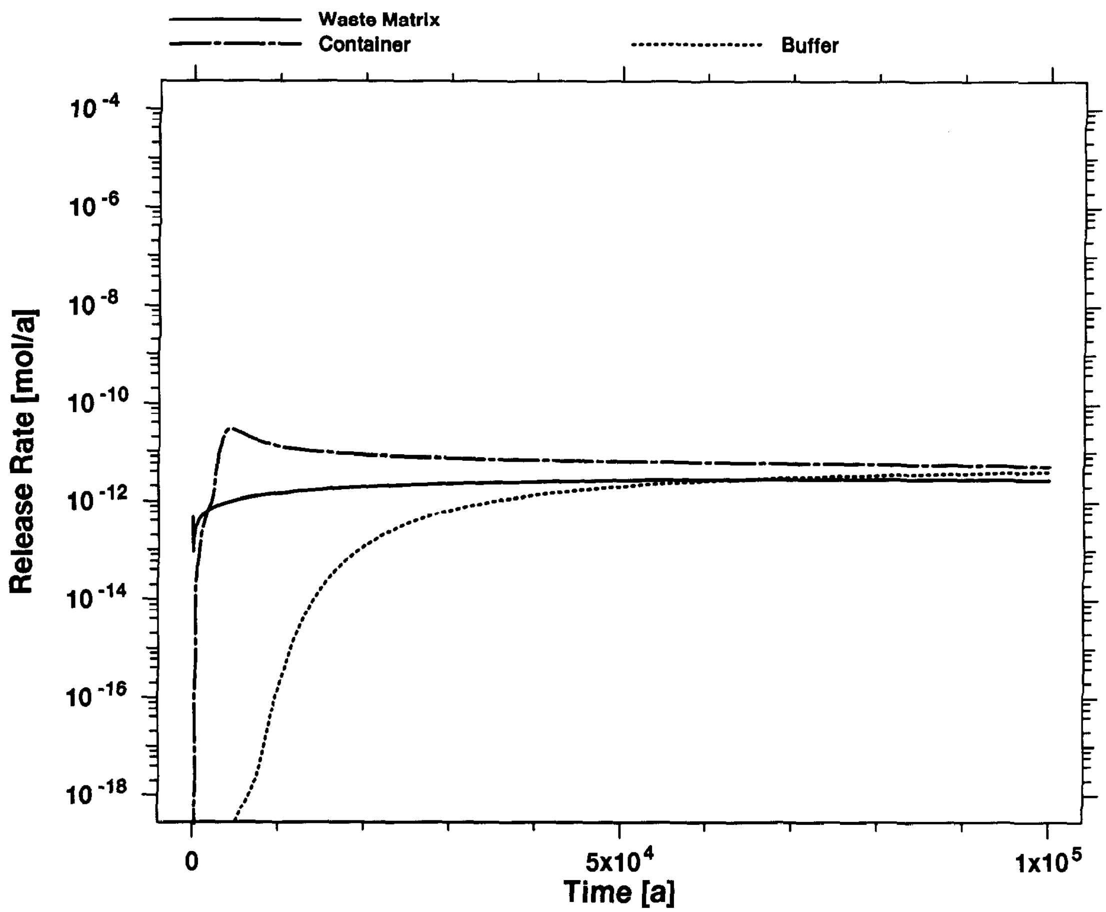

FIGURE D-11: Release Rates of ^{230}Th from Sector 11

This figure is similar to previous figures, except that it shows the results for ^{230}Th from the used-fuel matrix and using a logarithmic vertical scale. The three curves show, as a function of time, the rates of release of ^{230}Th from

(a) the used-fuel waste matrix,
(b) the containers, and
(c) the vault buffer.

The rate of release of ^{230}Th from the vault backfill to the rock surrounding sector 11 cannot be shown on this plot because the estimated values are less than 10^{-20} mol/a for all times up to 10^5 a. Thorium-230 releases are similar to those for ^{234}U and ^{238}U, except for the releases from the waste matrix. For the waste matrix (curve (a)), ^{230}Th releases first show a decrease resulting from decay, and then an increase resulting from ingrowth from its precursors.

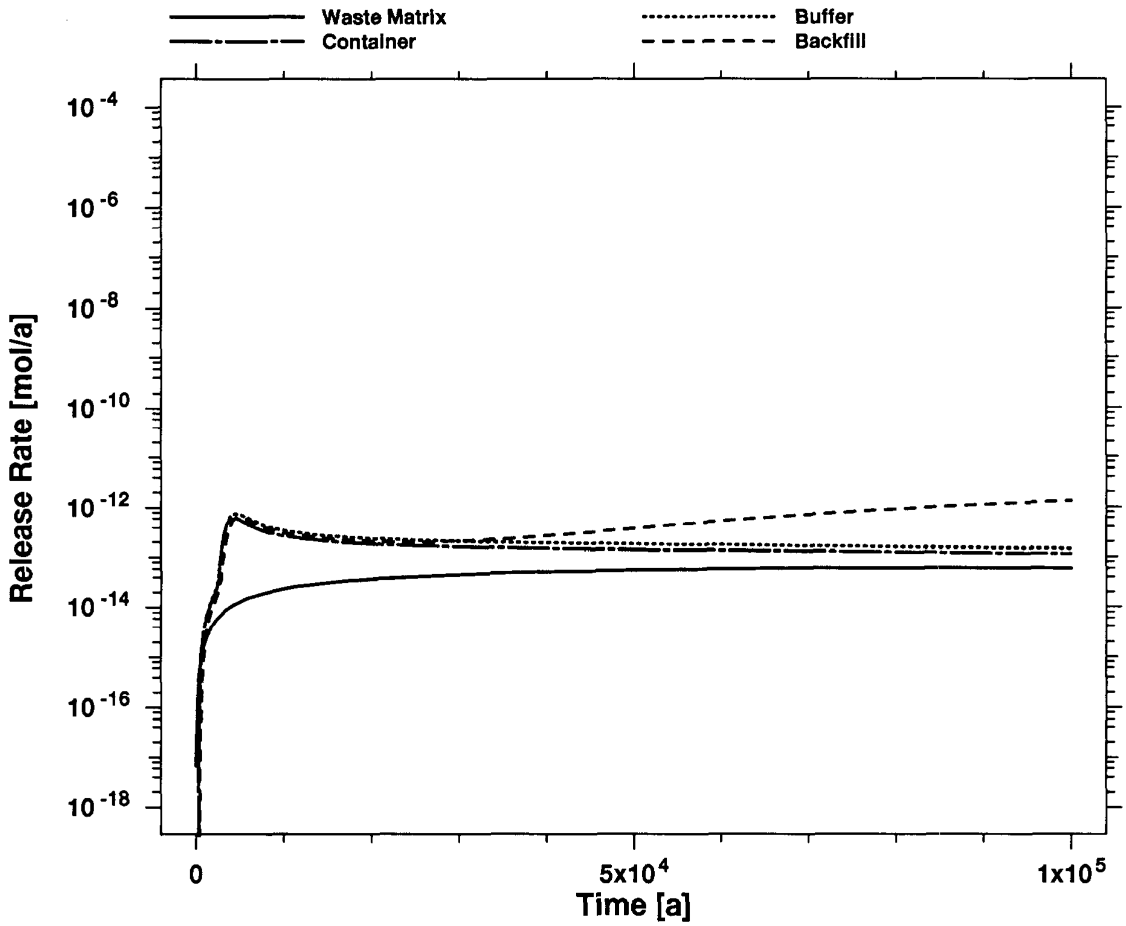

FIGURE D-12: Release Rates of ^{226}Ra from Sector 11

This figure is similar to previous figures, except that it shows the results for ^{226}Ra from the used-fuel matrix using a logarithmic vertical scale. The four curves show, as a function of time, the rates of release of ^{226}Ra from

(a) the used-fuel waste matrix,
(b) the containers,
(c) the vault buffer, and
(d) the vault backfill to the rock surrounding sector 11.

Radium-226 shows a slight increase in releases from the waste matrix because, like ^{230}Th, its inventory increases because of ingrowth from its precursors. Radium-226 is the only member of the ^{238}U decay chain with significant (but very small) releases from the backfill because it is only weakly sorbed onto the backfill and buffer.

There are no instant releases for members of the ^{238}U chain; consequently, their releases from the waste matrix are much smaller in magnitude than releases for ^{129}I and ^{14}C.

Figure D-9 shows the release rates for ^{238}U. Even though ^{238}U is the most abundant radionuclide in used fuel, its release from the used-fuel matrix is relatively small because of the small solubility of the used-fuel matrix (1.55×10^{-7} mol/m^3) in the chemical environment of the disposal vault (for the median-value simulation). Curve (a) of Figure D-9 shows that, although the ^{238}U initial release rate from the waste matrix is relatively large, it quickly drops below about 10^{-5} mol/a because its transport into the buffer is by diffusion:

- At first, there is a large concentration gradient between the containers and the buffer that enhances diffusive transport. Sorption on the buffer contributes to the maintenance of this large concentration gradient.

- Eventually ^{238}U concentrations in the buffer approach its (small) solubility limit and reduce the concentration gradient. Subsequently, the release rates show a gradual decline.

The ^{238}U release rate from the buffer is strongly attenuated and delayed because uranium is strongly sorbed onto the clay of the buffer. Releases from the buffer are insignificant for at least 10^4 a and reach a maximum at 10^5 a. (This corresponds to the end of the simulation time period; a global maximum would occur at even longer times.) Sorption in the backfill further delays and attenuates ^{238}U release. Moreover, the large capacity factor for ^{238}U in the backfill is such that insignificant quantities have left the backfill, even after 10^5 a.

Figure D-10 shows the release rates for ^{234}U. Its curves are similar to those in the previous figure for ^{238}U, principally because both radionuclides are isotopes of the same chemical element. The only major difference is that ^{234}U releases are about 4 orders of magnitude smaller than ^{238}U releases because the initial inventory of ^{234}U is about 4 orders of magnitude smaller.

Figures D-11 and D-12 show the release rates for ^{230}Th and ^{226}Ra. These radionuclides show slight increases in release rates from the waste matrix at longer times, primarily because of ingrowth from ^{234}U and ^{238}U. The sorption of ^{230}Th onto the buffer and backfill is the same as for uranium in the median-value simulation, and thus its releases are attenuated and delayed similar to the releases of the uranium isotopes.

In contrast, ^{226}Ra is weakly sorbed onto the buffer and backfill. Radium-226, therefore, moves more quickly through these media. Its release rate from the buffer reaches a maximum at a time only slightly later than its release rate from the containers. Radium-226 is the only chain member with a significant release rate from the backfill into the geosphere. The buffer and backfill release rates for ^{226}Ra show similar trends at early times, but more ^{226}Ra is released from the backfill at later times, reaching a maximum at 10^5 a, because of ingrowth from its precursors. However, the magnitude of the ^{226}Ra release rates are very small, less than

10^{-10} mol/a because its initial inventory is small and only small quantities are released from the used-fuel matrix and generated by ingrowth from its precursors.

D.2.6 SUMMARY OF RELEASES FROM THE VAULT IN 10^5 a

Table D-1 shows the amounts of eight contaminants in different parts of the vault for the median-value simulations. The other contaminants considered in the postclosure assessment have insignificant releases; typically of the order of 10^{-15} mol or less up to 10^5 a. The table shows that the largest releases are from ^{129}I and ^{14}C from the used-fuel matrix. As discussed earlier, the instant releases of these two contaminants are much more important than their congruent releases.

TABLE D-1

AMOUNTS OF EIGHT RADIONUCLIDES IN THE VAULT UP TO 10^5 a FOR THE MEDIAN-VALUE SIMULATION

Radio-nuclide	Initial Inventory (mol)	Amount in vault at 10^5 a (mol)	Vault Release to 10^5 a (mol)	Amount in Containers at 10^5 a (mol)	Amount in Buffer at 10^5 a (mol)	Amount in Backfill at 10^5 a (mol)
^{129}I	5.61×10^4	5.54×10^4	5.2×10^2	5.2×10^4	0.0	3.1×10^3
^{14}C	2.98×10^3	1.66×10^{-2}	1.8	1.5×10^{-2}	0.0	1.6×10^{-3}
^{14}C Z*	5.29×10^2	2.95×10^{-3}	3.5×10^{-7}	2.9×10^{-3}	0.0	6.5×10^{-10}
^{99}Tc	3.35×10^5	2.42×10^5	1.7×10^{-10}	2.3×10^5	1.5×10^4	1.2×10^{-1}
^{238}U	6.70×10^8	6.70×10^8	1.2×10^{-11}	6.7×10^8	4.2	8.3×10^{-3}
^{234}U	3.30×10^4	3.39×10^4	2.0×10^{-15}	3.4×10^4	2.1×10^{-4}	4.1×10^{-7}
^{230}Th	8.93×10^{-1}	6.27×10^3	1.1×10^{-14}	6.3×10^3	4.8×10^{-5}	9.8×10^{-6}
^{226}Ra	4.25×10^{-5}	1.28×10^2	3.4×10^{-6}	1.3×10^2	9.8×10^{-7}	3.0×10^{-8}

* ^{14}C Z is from the Zircaloy matrix. All other radionuclides are from the used-fuel matrix.

The second column of the table gives the initial inventory of the eight radionuclides. Columns 3 and 4 show the amounts remaining within the vault at 10^5 a and the amounts released to the geosphere up to 10^5 a. Column 2 is different from the sum of columns 3 and 4 because of radioactive decay: the last three radionuclides show an increase in mass because ingrowth from their precursors outweighs losses resulting from their own decay, whereas ^{14}C shows a loss because it has no precursors (and it has a relatively short half-life). The last three columns show the amounts remaining in the different parts of the vault. After 10^5 a, all containers have failed, and the values listed under amounts in the containers (column 5) include contaminants remaining in the waste matrices and in the void space within the containers.

Figures D-13 and D-14 show how much ^{129}I and ^{14}C have been released from the used-fuel matrix in each vault sector in the first 10^5 a after closure. The two figures represent the vault sectors as blocks, with the sector numbers indicated on each block.

- The location and area of the base of each block in the figure represent the location and area of the corresponding sector (compare with Figure D-1).

- The height of each block represents the release rate per unit area and is a measure of the relative effectiveness of each sector as a barrier. Most of the differences in effectiveness can be ascribed to the characteristics of the rock surrounding the sectors.

The volume of each block represents the total amount of ^{129}I or ^{14}C released by the corresponding sector in 10^5 a after vault closure. Figure D-13 indicates that sectors 1, 2 and 3 have the largest releases of ^{129}I, resulting mostly from their larger areas, and thus their larger initial inventories. Sectors 2 and 12 have the largest releases of ^{129}I per unit area, whereas sectors 4, 5, 10 and 11 have the smallest releases per unit area. Releases from sector 12 are greater than from sectors 10 and 11 because groundwater velocities in the rock surrounding sector 12 are higher, tending to more quickly transport ^{129}I away from that sector. However, we shall see in Section D.4 that releases from sector 11 dominate the radiological impacts.

The sum of all the sector releases, that is, the total amount released by the vault, is 519 mol for ^{129}I over 10^5 a, less than 1% of the total amount initially in the vault. The sum for ^{14}C is about 1.85 mol, or about 0.062% of its original inventory.

D.3 RESULTS FROM THE GEOSPHERE MODEL

The geosphere forms one of the major barriers isolating the contaminants in the vault from the biosphere. This section discusses, for the median case, the movement of contaminants leaving the vault and traversing this rock barrier. Section 5.4 in the main text describes the geosphere model, with more detail provided by Davison et al. (1994).

D.3.1 CHARACTERISTICS OF THE GEOSPHERE

Because the prevailing groundwater movement is generally toward the surface in the vicinity of the vault, the plume of contaminants will tend to move through the rock and the fracture zone above the vault, and proceed toward discharge zones in the biosphere. Thus the geosphere transport network is focussed on the region between the vault and the surface.

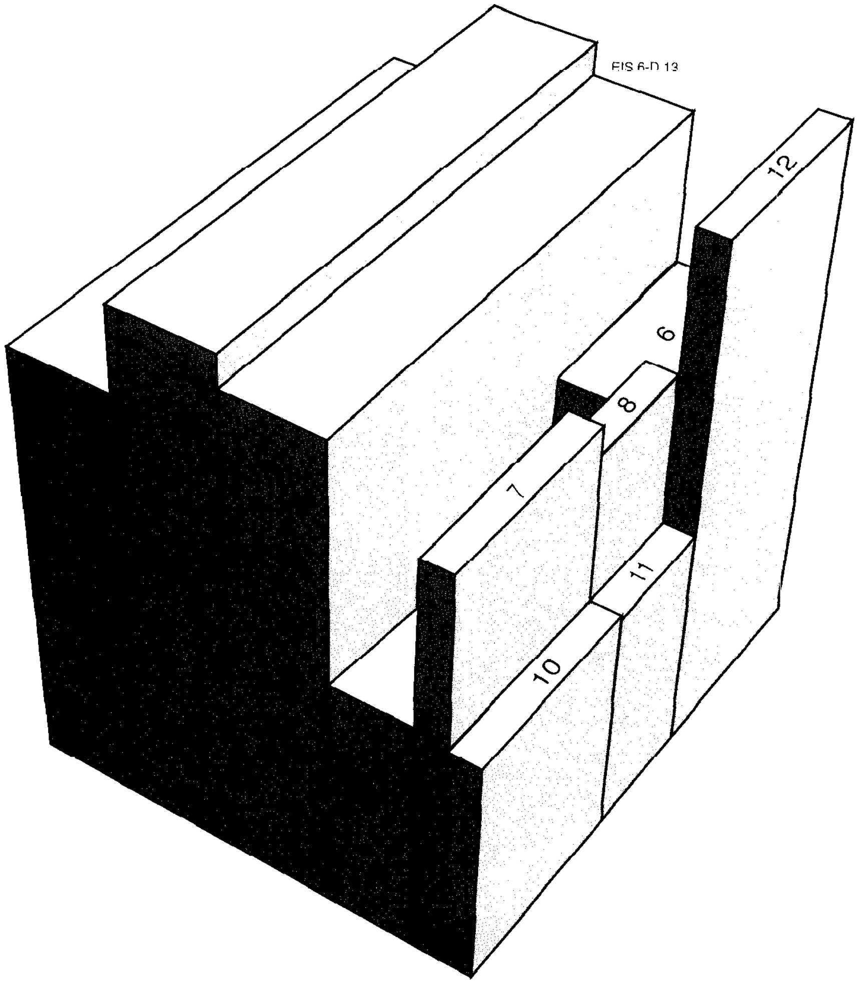

FIGURE D-13: Amount of ^{129}I Released from the Vault up to 10^5 a for the Median-Value Simulation

The blocks are labelled with the number of the corresponding vault sector, and their positions reflect the layout of the vault sectors (see Figure D-1). The height of a block is proportional to the amount of ^{129}I released per unit area up to 10^5 a, and the area of a block is proportional to the area of a vault sector. Thus the volume of a block is proportional to the total amount of ^{129}I released from a sector up to 10^5 a.

The total releases are largest for sectors 1, 2 and 3, whereas the per-unit-area releases are largest for sectors 2 and 12. Sector 12 shows a larger per-unit-area release than sectors 10 and 11 because of differences in groundwater velocities around these sectors (velocities are highest around sector 12).

The total release of ^{129}I from all sectors is about 519 mol in 10^5 a. About 123 mol are released from sector 1 and 17 mol from sector 12.

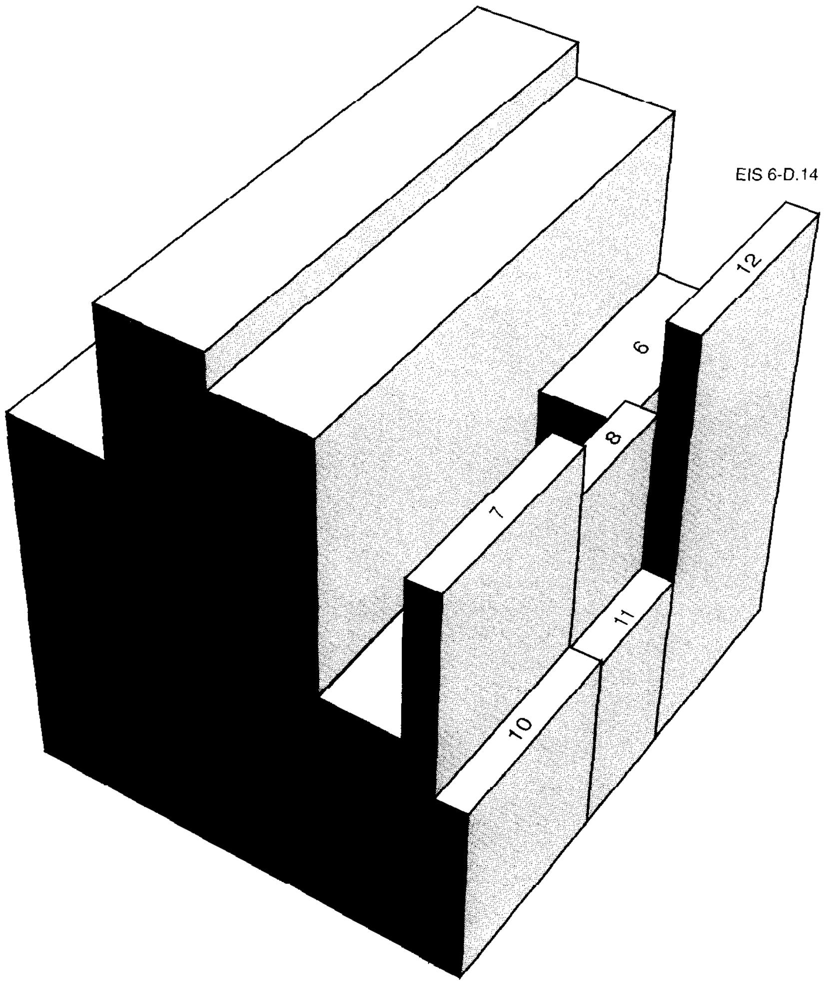

FIGURE D-14: Amount of ^{14}C Released from the Vault up to 10^5 a for the Median-Value Simulation

Comments are as for Figure D-13 except the data are for ^{14}C. The total release of ^{14}C from all sectors is about 1.85 mol in 10^5 a. About 0.40 mol are released from sector 1 and 0.054 mol from sector 12.

Table D-2 summarizes the important features of the geosphere for the median-value simulation. In the geosphere model, we assign unique properties to several different zones (Davison et al. 1994). These properties, which affect the movement of contaminants, include thickness, tortuosity (a measure of the increased distance for diffusive transport caused by the winding nature of the interconnected aqueous pathway), porosity, permeability and the minerals present (Section 5.4 of the main text). The different minerals present affect the degree of sorption of contaminants: quartz is relatively weakly sorbing, whereas goethite strongly sorbs most contaminants.

TABLE D-2

PROPERTIES OF IMPORTANT GEOSPHERE ROCK ZONES IN THE MEDIAN-VALUE SIMULATION[1]

	Lower Rock Zone	Middle Rock Zone	Upper Rock Zone	Fracture Zone LD1 (lower portion)	Overburden	Sediment
Physical Properties						
Thickness (m)	200	150	150	20	3.8	3.7
Porosity[2]	0.003	0.004	0.005	0.10	0.41	0.51
Tortuosity[2]	4.1	4.1	1.0	1.0	1.0	1.2
Dispersion length (m)	11	51	51	51	0.19	0.19
Permeability[3] (m^2)	1.0×10^{-19}	5.0×10^{-17}	5.0×10^{-15}	1.0×10^{-13}	2.1×10^{-14}	1.1×10^{-12}
Typical groundwater velocity (m/a)	5.9×10^{-6}	4.3×10^{-3}	1.5	1.3	0.019	0.015
Groundwater Chemistry						
Salinity of groundwater (kg/m^3)	20.0	8.0	0.55	12.5	0.55	0.55
Mineral Fractions of the Rock and Overburden[4]						
Grey granite	1.0	1.0	0.0	0.0	0.0	0.0
Biotite	0.0	0.0	0.0	0.05	0.0	0.0
Calcite	0.0	0.0	0.30	0.03	0.0	0.0
Chlorite	0.0	0.0	0.25	0.14	0.0	0.0
Goethite	0.0	0.0	0.30	0.15	0.0	0.0
Illite	0.0	0.0	0.02	0.19	0.0	0.0
Microcline	0.0	0.0	0.03	0.15	0.0	0.0
Muscovite	0.0	0.0	0.0	0.03	0.0	0.0
Plagioclase	0.0	0.0	0.05	0.11	0.0	0.0
Quartz	0.0	0.0	0.05	0.15	0.0	0.0
Clay	0.0	0.0	0.0	0.0	0.50	0.0
Silt	0.0	0.0	0.0	0.0	0.23	0.0
Sand	0.0	0.0	0.0	0.0	0.27	0.0
Organic	0.0	0.0	0.0	0.0	0.0	1.0

continued...

TABLE D-2 (concluded)

	Lower Rock Zone	Middle Rock Zone	Upper Rock Zone	Fracture Zone LD1 (lower portion)	Overburden	Sediment
Retardation Factors[5]						
Americium	32000	32000	3900	10000	20000	34000
Cadmium	41	41	48	44	940	240
Carbon	1.0	1.0	100.	11	19	22
Cesium	2400	2300	63	88	5780	83
Iodine	1.0	1.0	1.0	1.0	6.3	8.6
Plutonium	1100	1100	1300	2300	8900	580
Radium	700	700	360	5700	35000	730
Samarium	2500	2500	820	300	2600	910
Selenium	110	130	120	90	1500	550
Technetium	2.6	2.6	12	45	2.7	1.3
Thorium	3200	3200	3800	3400	14000	27000
Uranium	24	24	3200	920	2400	130
Zirconium	9600	9600	1100	10000	6800	2200

1 The geosphere model includes physical and chemical properties of different rock zones that may lie in the flow path of the contaminants. This table gives representative values for these properties, for six of the more important rock zones.

2 Tortuosity and porosity have dimensionless units.

3 Permeabilities can be different in different directions. The values given for the lower, middle and upper rock zones are in the vertical direction; permeabilities in the horizontal direction are about 5 times smaller. The value given for LD1 is in the plane of LD1; its permeability in a transverse direction is a factor of 2 smaller.

4 Numbers shown are the fractions of different minerals in each rock zone.

5 Retardation Factors combine the chemical properties with some of the physical properties to give examples of the degree of sorption of contaminants in the rock zones. A large retardation factor means that a contaminant is strongly sorbed and moves much more slowly than groundwater. The minimum retardation factor is unity; it occurs when a contaminant moves at the same velocity as the groundwater.

The data in Table D-2 indicates that the geosphere model explicitly incorporates a wide range of properties; for example,

- permeabilities range over 7 orders of magnitude;

- mineral compositions of the rock range from undifferentiated grey granite to fracture infilling minerals such as calcite, chlorite and goethite; and

- retardation factors can vary by more than 2 orders of magnitude for a single chemical element in different rock zones and by more than 4 orders of magnitude for different chemical elements in a single rock zone.

Four of the more important zones in the geosphere model are

- The lower rock zone (layer 3 in Figures 5-12 and 5-13 in the main text) that surrounds the vault. Groundwater velocities tend to be so low that contaminant transport is dominated by diffusion. The most abundant mineral is grey granite, and contaminant sorption ranges from small to large values. ("Grey granite" is actually a rock and not a mineral. We use this name to identify a hypothetical mineral with composite sorptive properties.)

- Fracture zones that pass through the rock in the geosphere, particularly fracture zone LD1 (Figure D-15). Groundwater velocities in LD1 are relatively high, and contaminant transport by moving groundwater is dominant. Contaminant sorption can be significant, largely because of the presence of the reactive minerals found in fracture zones.

- The upper rock zone, lying immediately below the surface overburden (layer 1 in Figures 5-12 and 5-13 in the main text). Groundwater velocities are typically high, and contaminant transport in moving groundwater is more important than diffusion. This zone is intersected by a number of subvertical fractures, thus groundwater movement is directed upwards rather than horizontally. These fractures also contain large amounts of calcite, chlorite and goethite, which tend to have good capabilities for contaminant sorption.

- The overburden zone that lies under the soil and lake sediment (and is considered to be a part of the geosphere model in our studies). This zone is relatively porous, and groundwater velocities are not high. However, it is shallow, so that groundwater transit times through it are not long. The overburden consists largely of clay, and thus it tends to have substantial capabilities for contaminant sorption.

Contaminant transport through the geosphere is simulated using a network of geosphere segments. As discussed in Chapter 5 of the main text, there are 46 segments in the geosphere model, including 12 that connect with the 12 vault sectors, and 4 that connect with the 4 discharge zones in the biosphere. Figure D-15 illustrates this network of segments and shows the

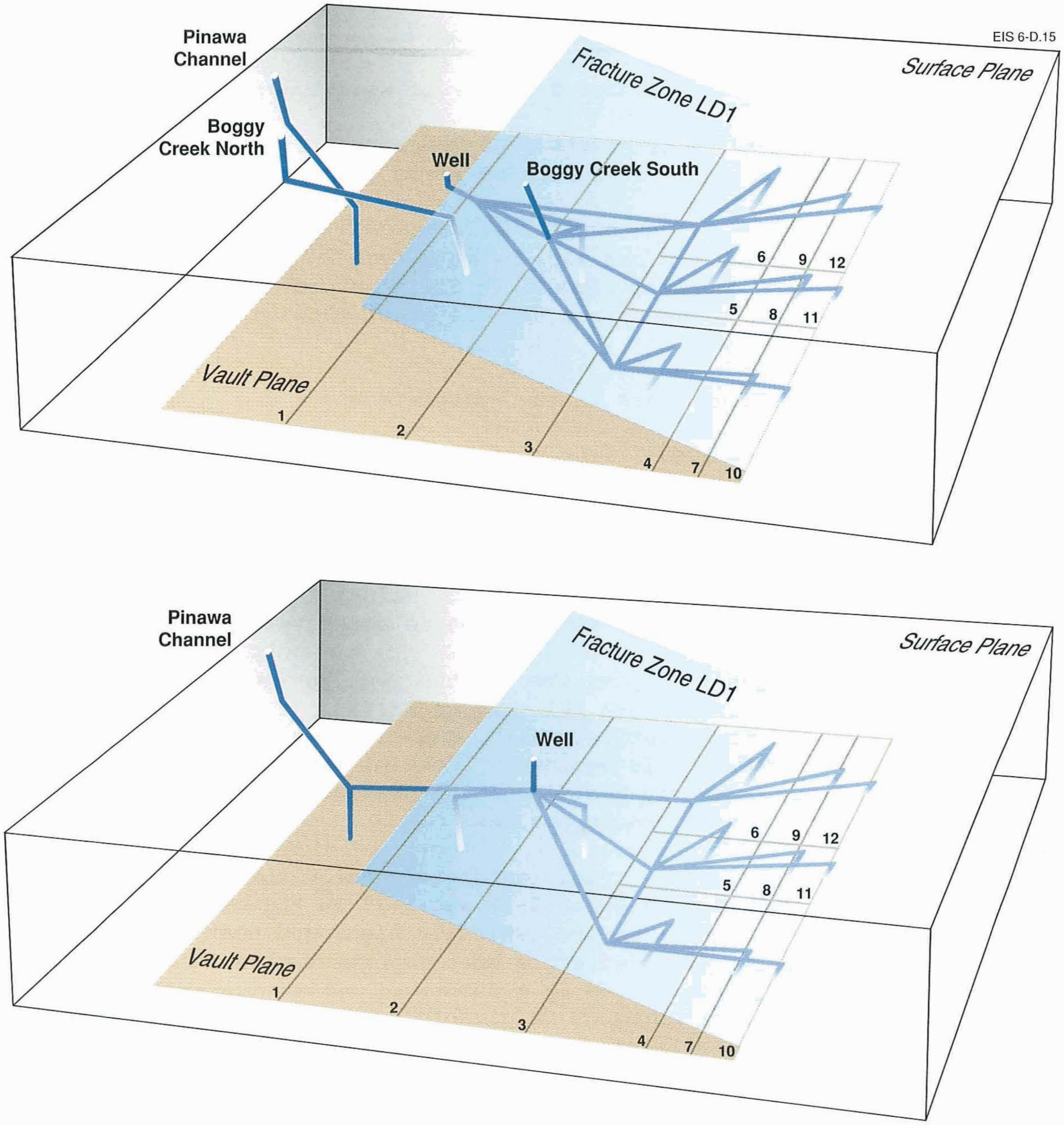

FIGURE D-15: Illustration of the Network Segments in the Geosphere Model

Contaminants leave the vault through 12 nodes lying in the vault plane, then pass from segment to segment until they reach one of the 4 discharge zones in the surface plane: Pinawa Channel, Boggy Creek North, Boggy Creek South and the well. The top figure shows the segment used in the median-value simulation, where the bedrock well is 37 m deep. Fracture zone LD1 captures the contaminants leaving vault sectors 3 through 12 and leads to discharges at the well and Boggy Creek South. The bottom figure shows segments used for sensitivity analyses involving a deep (200 m) bedrock well and large well demands, where the well captures all the contaminants leaving sectors 2 to 12 and some of the contaminants leaving sector 1; in addition, the well captures the discharges leading to Boggy Creek South.

complex pattern of groundwater movement that is represented in the geosphere model (see also Figure 5-14 in the main text).

The properties of each segment are partly determined by the properties of the rock zones in which they are found. One important property is the groundwater velocity in a segment, which is determined by permeability, porosity and pressure difference (or hydraulic head). Groundwater velocities are low in segments in the lower rock zone because permeabilities and pressure differences are low. The properties in fracture zone LD1 are different, and velocities are greater. Table D-3 summarizes the properties of some representative segments and illustrates the wide range of geosphere properties included in the network of segments.

Another property of each segment can be summarized using a dimensionless factor analogous to the Peclet number (Bear 1975), which we refer to below as the diffusive Peclet number. We define the diffusive Peclet number for a segment as the expression

$$\frac{V \cdot L}{D_e}$$

where, for each segment, V is the groundwater velocity, L is the characteristic length, and D_e is the effective diffusion coefficient. The literature describes a number of different possible choices for these three parameters. We use the groundwater velocity in the segment, the geometric distance between the nodes defining the start and end of the segment, and the free-water diffusion coefficient divided by the square of the tortuosity of the segment.

Contaminant transport times by diffusion are of the order of L^2/D_e, whereas transport times in moving groundwater are of the order L/V. Thus the definition given above is the ratio of transport times by diffusion to transport times in moving groundwater. For this ratio

- Large values (greater than about 5) mean the movement of nonsorbing contaminants will be dominated by transport in flowing groundwater (because transport times by diffusion are greater than transport times in moving groundwater),

- Small values (less than about 0.5) mean that diffusive transport dominates, and

- Intermediate values mean that both transport mechanisms are important.

Table D-3 includes diffusive Peclet numbers. The results lead to the conclusions:

- Diffusion dominates contaminant transport for segments in the lower rock zone, such as segment number 12 that leads from vault sector 11 to fracture zone LD1;

- Moving groundwater dominates contaminant transport in all segments along fracture zone LD1, such as segment number 35; and

TABLE D-3

TRANSPORT PROPERTIES OF REPRESENTATIVE SEGMENTS

IN THE MEDIAN-VALUE SIMULATION

Representative Segment Number[1]	#12	#51	#52	#35	#56	#57
	Lower Rock Zone	Middle Rock Zone	Upper Rock Zone	Fracture Zone LD1 (lower portion)	Overburden	Sediment
Transport Property						
Segment length (m)	46.5	355	155	536	3.77	3.66
Groundwater velocity (m/a)	0.0000059	0.0043	1.50	1.30	0.019	0.015
Groundwater transit time (a)	7 800 000	83 000	100	430	200	240
Diffusion coefficient[2] (m^2/a)	0.047	0.047	0.047	0.047	0.047	0.047
Dispersion length (m)	10.5	50.5	50.5	50.5	0.186	0.186
Dispersion coefficient (m^2/a)	0.0030	0.22	77.	64.	0.051	0.035
Diffusive Peclet number[3]	0.10	550.	5000	14 000	1.5	1.7

1 Data shown are from segments that lie within the rock zones characterized in Table D-2. The segment number corresponds to that number used in SYVAC3-CC3 to identify segments in the geosphere model (see Figure D-15).

2 All elements have the same value for the free-water diffusion coefficient.

3 The diffusive Peclet number (defined in the text) is a dimensionless ratio that indicates the dominant transport process for a nonsorbing contaminant. Values greater than about 5 indicate transport in moving groundwater is most important, and values less than about 0.5 indicate transport by diffusion is most important.

- Both diffusion and moving groundwater affect contaminant transport in the overburden and sediment segments.

The properties of the geosphere are such that, after 10^5 a following closure, only extremely small amounts of contaminants could reach the discharges in the Pinawa Channel and the north part of Boggy Creek. The two more important discharge areas are the south part of Boggy Creek and the well, because both are connected to fracture zone LD1. Once a contaminant has entered LD1, it travels relatively quickly. Contaminants that do not sorb strongly, such as ^{129}I, move the length of LD1 in about 1000 a.

In the median-value simulation, the well intersects fracture zone LD1 at a depth of 37 m and supplies a total of 1330 m^3 water per year. This well demand causes a reduction (drawdown) in the hydraulic head by 4.8 m at the well and by less than 0.1 m in the fracture zone at the level of the vault. With this depth and drawdown, the well captures about 40 m^3/a surface water from Boggy Creek. The remaining 1290 m^3/a is deep groundwater from LD1.

This deep groundwater includes 31% of the contaminant plume travelling up LD1 (mostly originating from vault sector 11). The remaining 69% of the plume in LD1 (mostly from vault sectors 10 and 12) discharges to the South portion of Boggy Creek after passing through the upper rock zone, 3.8 m of overburden and 3.7 m of organic sediment.

D.3.2 MOVEMENT OF CONTAMINANTS IN THE GEOSPHERE

We examine in this section how the characteristics of the geosphere affect the movement of contaminants from the vault. As discussed previously in Figure D-13, the releases of contaminants from the vault are greatest from vault sectors 1, 2 and 3, which are remote from fracture zone LD1. However, their transport paths (segments) to the surface are long, and movement is slow; they do not significantly contribute to the release of contaminants to the biosphere. Instead, the contaminants from these sectors remain in the rock, moving slowly toward the surface discharges in Pinawa Channel and Boggy Creek.

The releases from vault sectors 10, 11 and 12, which are nearest fracture zone LD1, have relatively short transport paths to the fracture zone, so that transport is relatively fast. We shall see below that these sectors contribute the bulk of the contaminants entering the biosphere for times up to 10^5 a after closure.

We conclude that the most important barrier within the geosphere representing the disposal site considered in this postclosure assessment study is the low-permeability sparsely fractured rock surrounding the vault. Figures D-16 to D-18 illustrate its effect in delaying and attenuating transport of ^{129}I, ^{14}C and ^{99}Tc. The three figures show

- the rates of release of ^{129}I, ^{14}C and ^{99}Tc from vault sector 11; and

- their subsequent rates of arrival at fracture zone LD1.

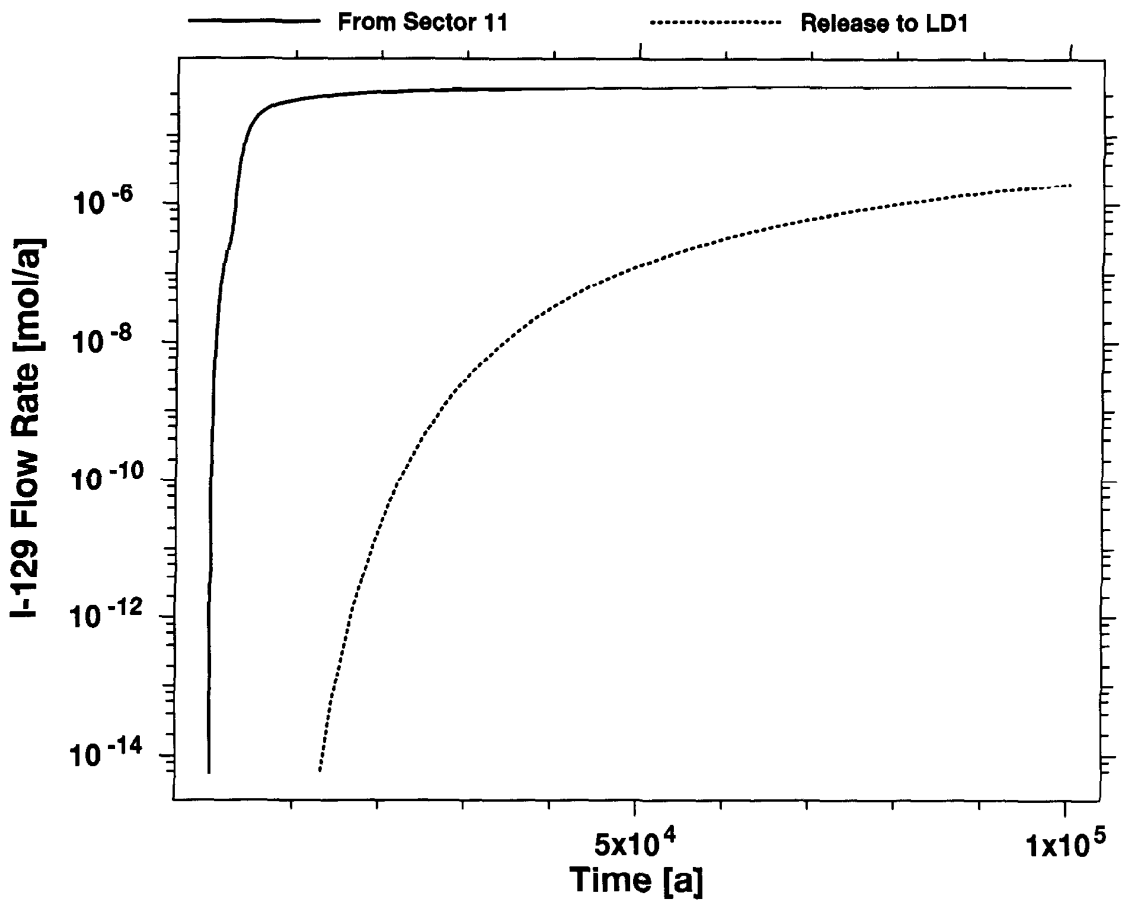

FIGURE D-16: The Effect of the Lower Rock Zone on ^{129}I Transport

The two curves illustrate, for ^{129}I

- its rate of release from vault sector 11, and
- its subsequent rate of arrival at fracture zone LD1.

The delay and attenuation in ^{129}I at LD1 is due to its transport through the waste exclusion distance, consisting of about 50 m of sparsely fractured gray granite in the lower rock zone. Note that the vertical axis uses a logarithmic scale to span a large range of transport rates.

There is about 50 m of highly impermeable, sparsely fractured granite separating sector 11 from LD1; this barrier delays any significant arrival of ^{14}C and ^{129}I for more than 10^4 a. Technetium is delayed even more because it sorbs onto the minerals found in the lower rock zone.

We chose vault sector 11 for these figures because it has the shortest segment length in the lower rock zone (about 50 m) and because contaminants from this sector dominate radiation doses (discussed in Section D.4). Part of the reason for this domination of the impacts is shown in Figures D-19 to D-22.

Figure D-19 summarizes the releases of ^{129}I from the lower rock zone up to 10^5 a:

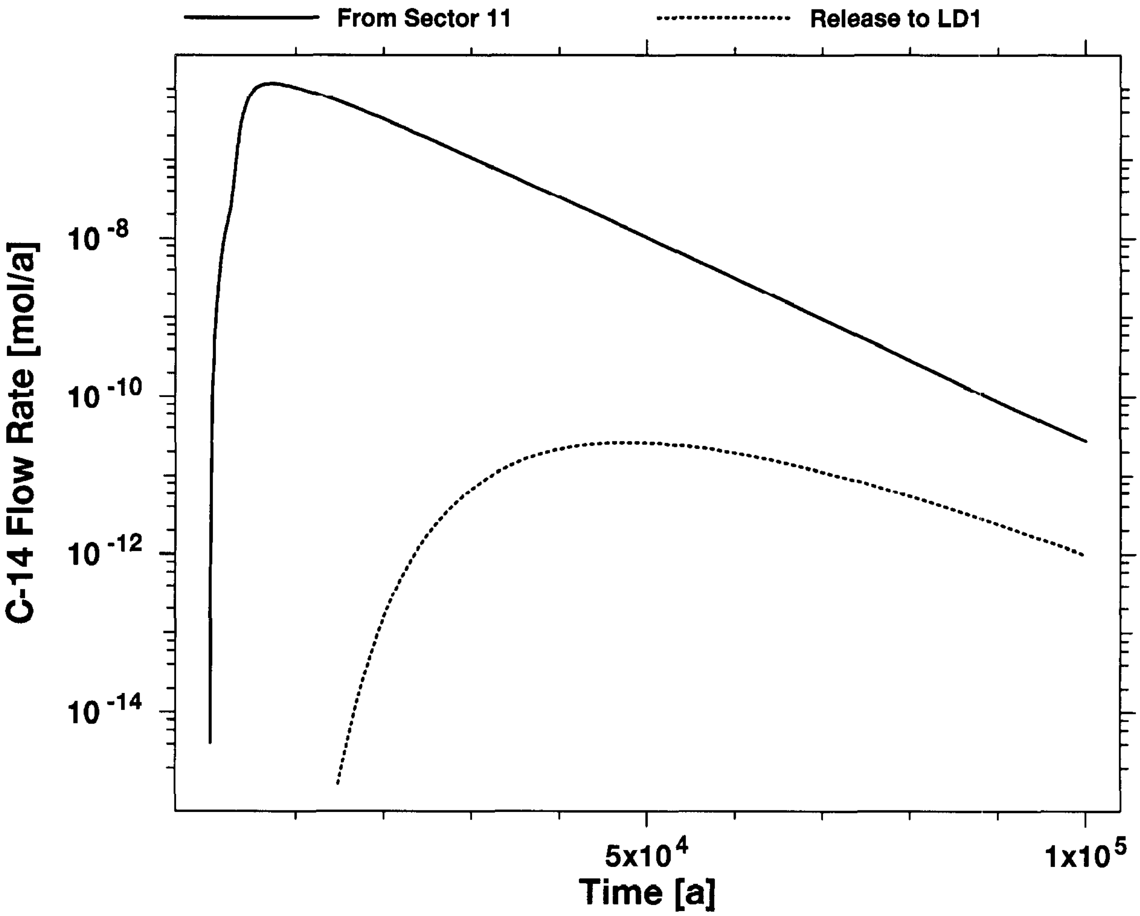

FIGURE D-17: The Effect of the Lower Rock Zone on ^{14}C Transport

The two curves illustrate, for ^{14}C
- its rate of release from vault sector 11, and
- its subsequent rate of arrival at fracture zone LD1.

The delay and attenuation in ^{14}C at LD1 is due to its transport through the waste exclusion distance, consisting of about 50 m of sparsely fractured gray granite in the lower rock zone. Both curves show a maximum because the effects of its radioactive decay are more important at longer times, reducing ^{14}C inventory (and transport rates). Note that the vertical axis uses a logarithmic scale to span a large range of transport rates.

- It is clear that most of the ^{129}I releases originate from vault sectors 10, 11 and 12. Contaminant transport from these sectors through the adjoining lower rock zone is dominated by diffusion, with a (relatively short) path length of about 50 m.

- Releases originating from the sectors at the other end of the vault are much smaller. For example, the transport distance is 200 m from vault sector 1 to the intermediate rock zone. Consequently, transport times are so long that no ^{129}I passes through the lower rock zone from sector 1, even in 10^5 a following vault closure.

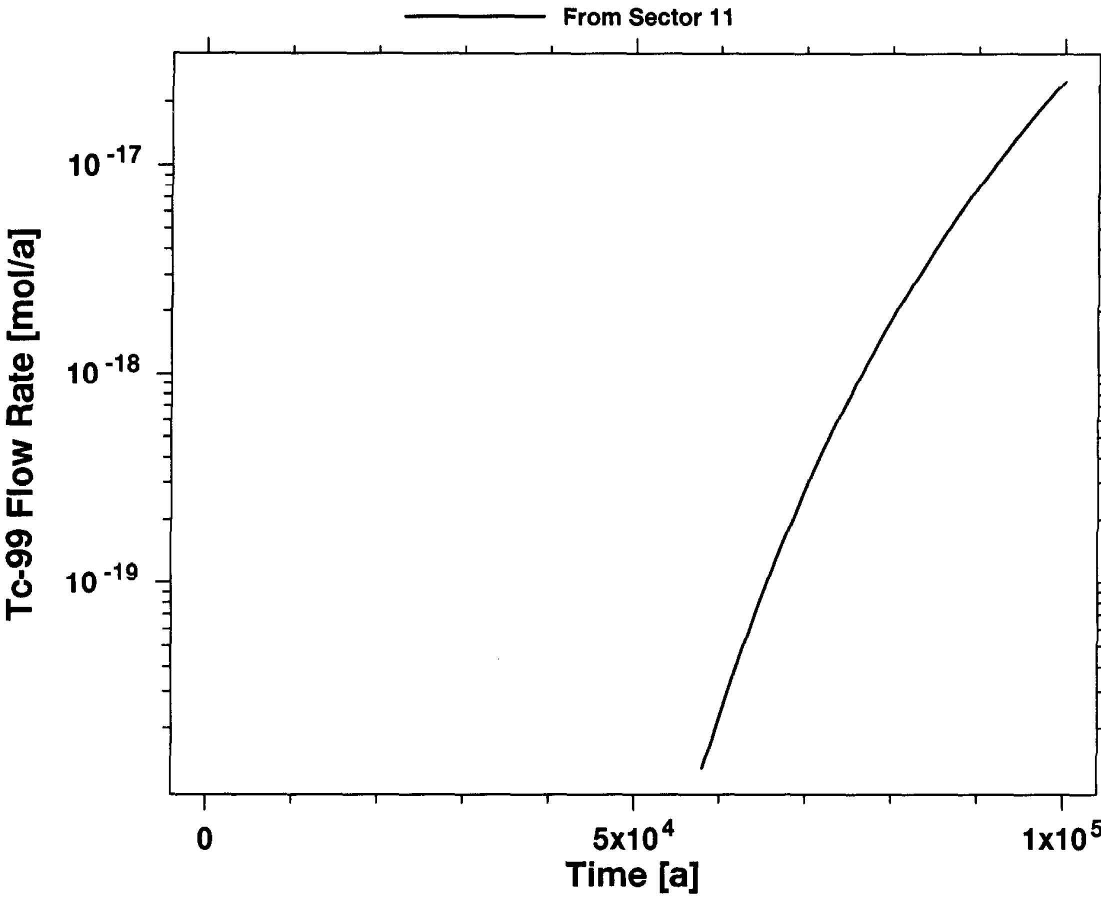

FIGURE D-18: The Effect of the Lower Rock Zone on ^{99}Tc Transport

There is only one curve, giving the rate of release of ^{99}Tc from vault sector 11. The transport rates involved are slow, less than 10^{-15} mol/a for times up to 10^5 a. The subsequent transport of ^{99}Tc in the lower rock zone is slow; for all practical purposes no ^{99}Tc reaches fracture zone LD1. Note that the vertical axis has a logarithmic scale to span a large range of transport rates.

Figure D-20 shows the amount of ^{14}C released from the lower rock zone. Again, most of the ^{14}C releases in 10^5 a originate from vault sectors 10, 11 and 12.

The only significant discharge of contaminants from the geosphere occurs at the well and Boggy Creek South because both are connected to fracture zone LD1 (Figure D-15). Figures D-21 and D-22 illustrate for ^{129}I and ^{14}C respectively the contributions to these discharges from the 12 vault sectors.

- Releases that originate from vault sector 11 dominate the discharges to the well.

- Releases from vault sectors 10 and 12 dominate the discharges to Boggy Creek South.

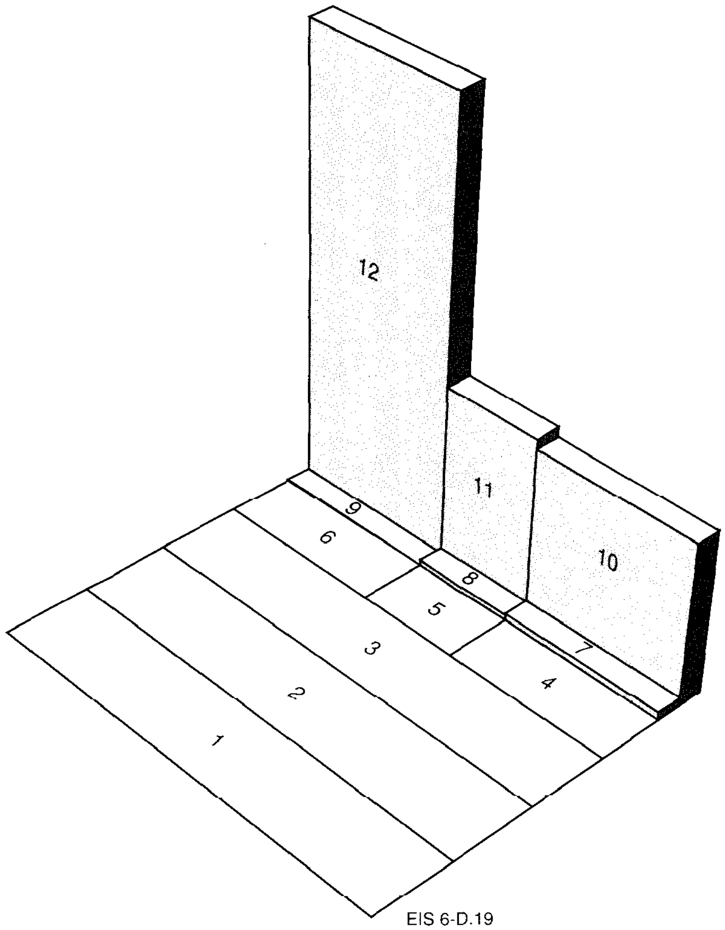

FIGURE D-19: Amount of ^{129}I Released from the Lower Rock Zone up to 10^5 a

Each block represents a segment in the geosphere model that starts from a vault sector and traverses the adjacent rock in the lower rock zone. The blocks are labelled with the number of the corresponding vault sector, and the block locations reflect the layout of the vault sectors (Figure D-1 in Section D.1). The height of the blocks is proportional to the amount of ^{129}I released from each segment per unit area up to 10^5 a. The area of each block corresponds to the area of the vault sector adjoining the segment. The volume of each block is then proportional to the total amount of ^{129}I released from each segment up to 10^5 a.
The total release of ^{129}I from these segments is 0.32 mol in 10^5 a. Most of the release (0.20 mol) comes from vault sector 12 and enters the fracture zone that directly adjoins the segment connected to that sector. (Compare with Figures D-13 and D-21.)

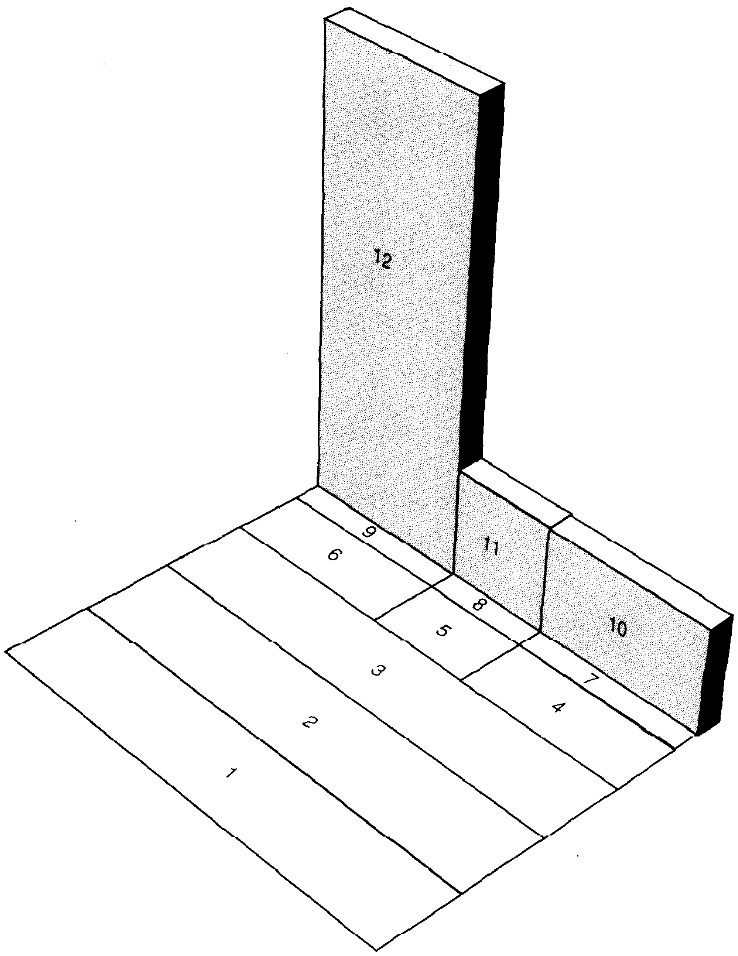

FIGURE D-20: Amount of ^{14}C Released from the Lower Rock Zone up to 10^5 a

Each block represents a segment in the geosphere model, which starts from a vault sector and traverses the adjacent rock in the lower rock zone. The blocks are labelled with the number of the corresponding vault sector, and the block locations reflect the layout of the vault sectors (Figure D-1). The height of the blocks is proportional to the amount of ^{14}C released from each segment per unit area up to 10^5 a. The area of each block corresponds to the area of the vault sector adjoining the segment. The volume of each block is then proportional to the total amount of ^{14}C released from each segment up to 10^5 a.
The total release of ^{14}C from these segments is about 0.08 mol in 10^5 a. Most of the release comes from vault sector 12 and enters the fracture zone that directly adjoins the segment connected to that sector. (Compare with Figures D-14 and D-22.)

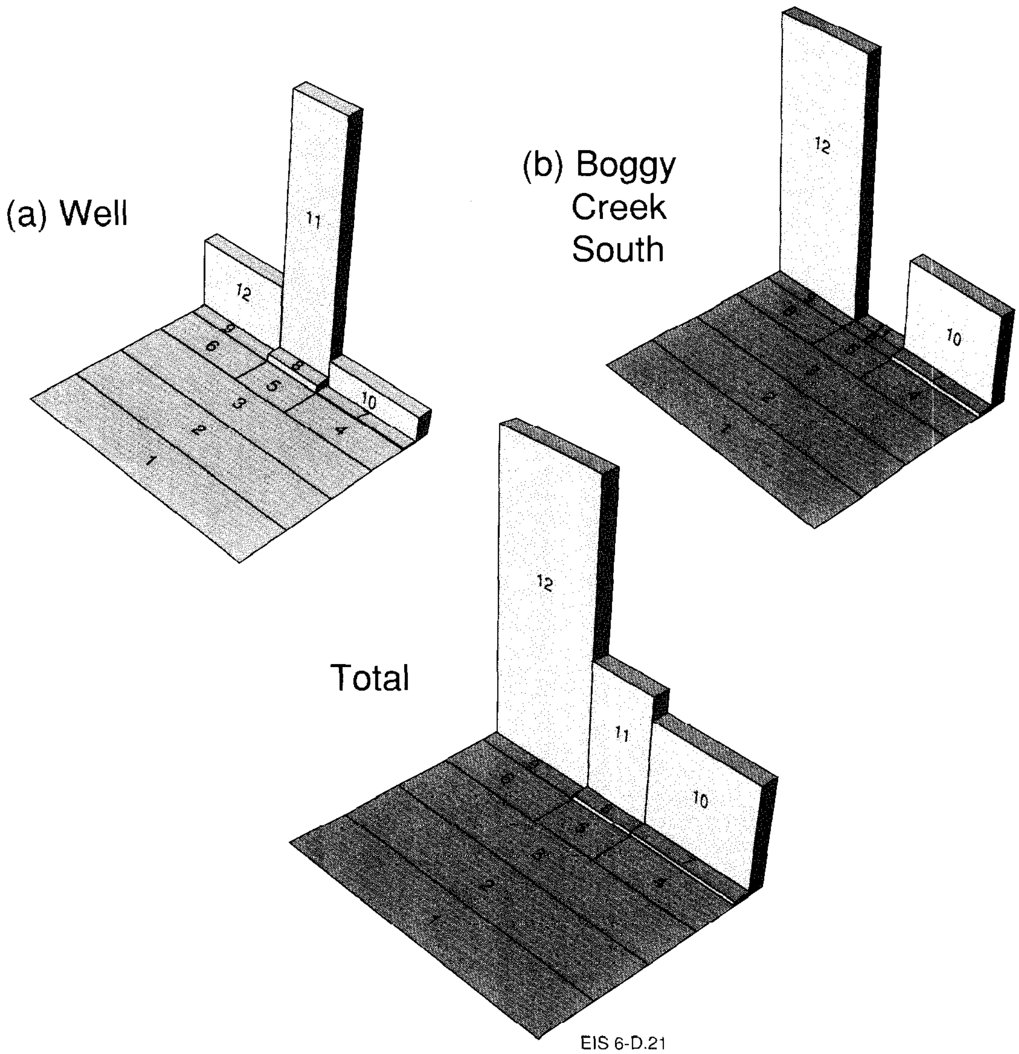

FIGURE D-21: Amount of ^{129}I Discharged to the Biosphere up to 10^5 a

Part (a) shows discharges to the well, part (b) to Boggy Creek South, and the figure labelled "Total" is the sum of (a) and (b). For parts (a) and (b), each block represents the discharge contributions from a vault sector. The blocks are labelled with the number of the vault sector connected to the segment, and the block locations reflect the layout of vault sectors. The volume of each block is proportional to the total amount of ^{129}I discharged to the biosphere up to 10^5 a.

The well captures all of the ^{129}I that was released from vault sector 11, along with some of the releases from sectors 10 and 12. The bulk of the releases from sectors 10 and 12 discharge to Boggy Creek South. The other vault sectors do not contribute or make small contributions. (Compare with Figures D-13 and D-19.)

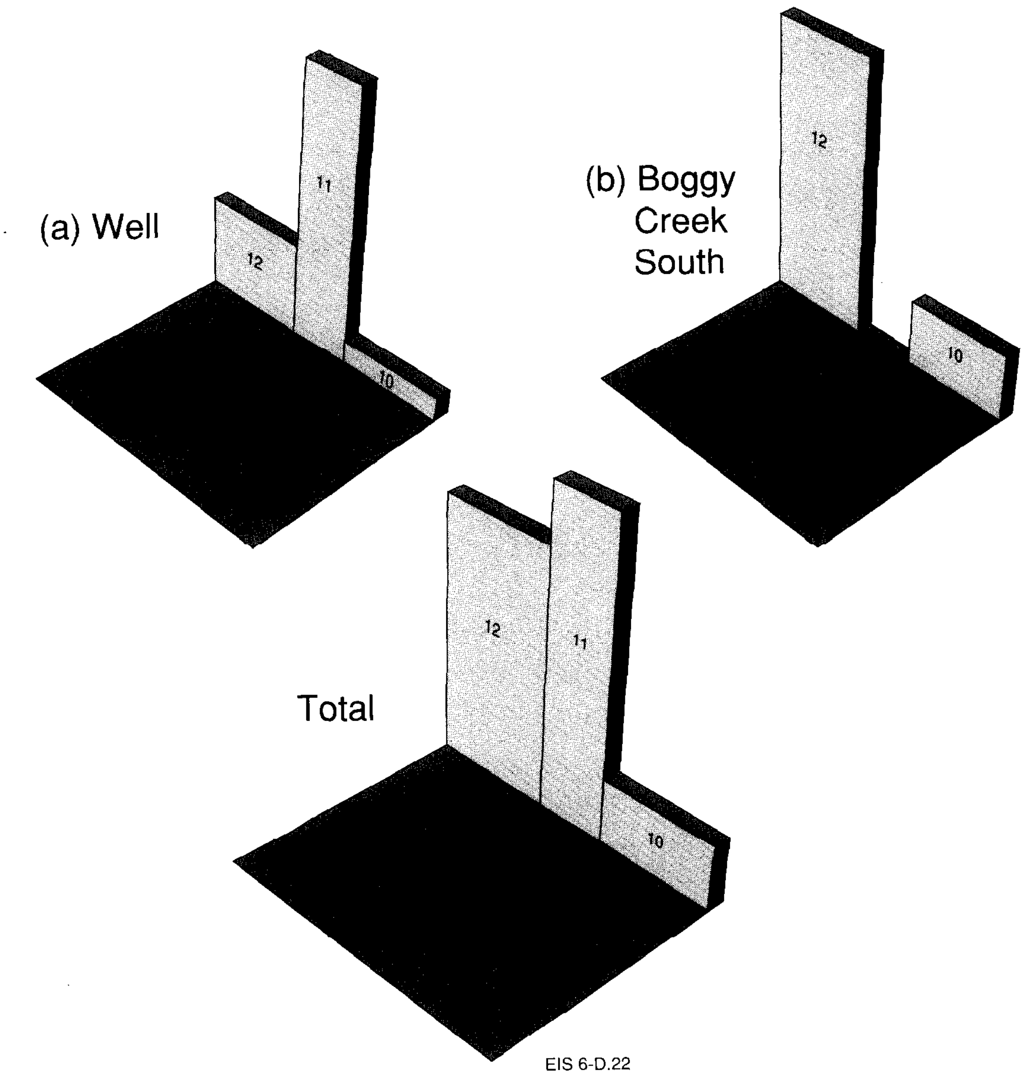

FIGURE D-22: Amount of ^{14}C Discharged to the Biosphere up to 10^5 a

Part (a) shows discharges to the well, part (b) to Boggy Creek South, and the figure labelled "Total" is the sum of (a) and (b). For parts (a) and (b), each block represents the discharge contributions from a vault sector. The blocks are labelled with the number of the vault sector connected to the segment, and the block locations reflect the layout of vault sectors. The volume of each block is proportional to the total amount of ^{14}C discharged to the biosphere up to 10^5 a.
The well captures all the ^{14}C that was released from vault sector 11, along with some of the releases from sectors 10 and 12. The bulk of the releases from sectors 10 and 12 discharge to Boggy Creek South. The other vault sectors do not contribute or make small contributions. (Compare with Figures D-14 and D-20.)

- Releases from vault sectors 1, 2 and 3 do not contribute because they are not connected to LD1.

- Releases from sectors 4 through 9 contribute negligible amounts, even after 10^5 a.

The discussion in Section D.4 will show that most of the estimated radiation doses are associated with the well and, therefore, with releases that originate from vault sector 11.

D.3.3 DISTRIBUTION OF CONTAMINANTS IN THE GEOSPHERE

Figure D-23 shows the distribution of ^{129}I in the disposal system after 10^5 a. The initial inventory of ^{129}I is 56 100 mol (7240 kg), and

- 98.6% is still in the vault;

- About 0.925% (520 mol, or 67 kg) is travelling through the lower rock zone;

- 0.0001% (about 0.06 mol, or 7 g) is travelling through the remainder of the geosphere, including LD1 and overburden;

- Less than 0.0005% (0.28 mol, or 36 g) has entered the biosphere over times up to 10^5 a: about one quarter through the well and three quarters to Boggy Creek South.

- The rest of the ^{129}I, about 0.44%, has undergone radioactive decay.

Figure D-24 shows the distribution of ^{14}C in the disposal system after 10^5 a. The initial inventory of ^{14}C is 2980 mol (41.7 kg), and

- Most of the initial inventory of ^{14}C no longer exists in the disposal system because of radioactive decay: 99.94% decays in the vault and most of the remainder decays in the lower rock zone;

- About 3×10^{-9}% is retained in the geosphere above the lower rock zone.

- Only small quantities of ^{14}C survive to reach the biosphere. As shown in Figure D-24, about 3×10^{-8}% is discharged to the biosphere, about twice as much through the well as through Boggy Creek South. (As noted in Section D.2, recent data for the instant-release fraction for ^{14}C (Johnson et al. (1994) indicate that we have overestimated the release of ^{14}C from the disposal vault and, therefore, overestimated the amount that would arrive at the biosphere).

Figure D-25 shows the distribution of ^{99}Tc in the disposal system after 10^5 a. The initial inventory of ^{99}Tc is 335 000 mol (33 200 kg), and

- 72% (241 000 mol, or 23 900 kg) is still in the vault;

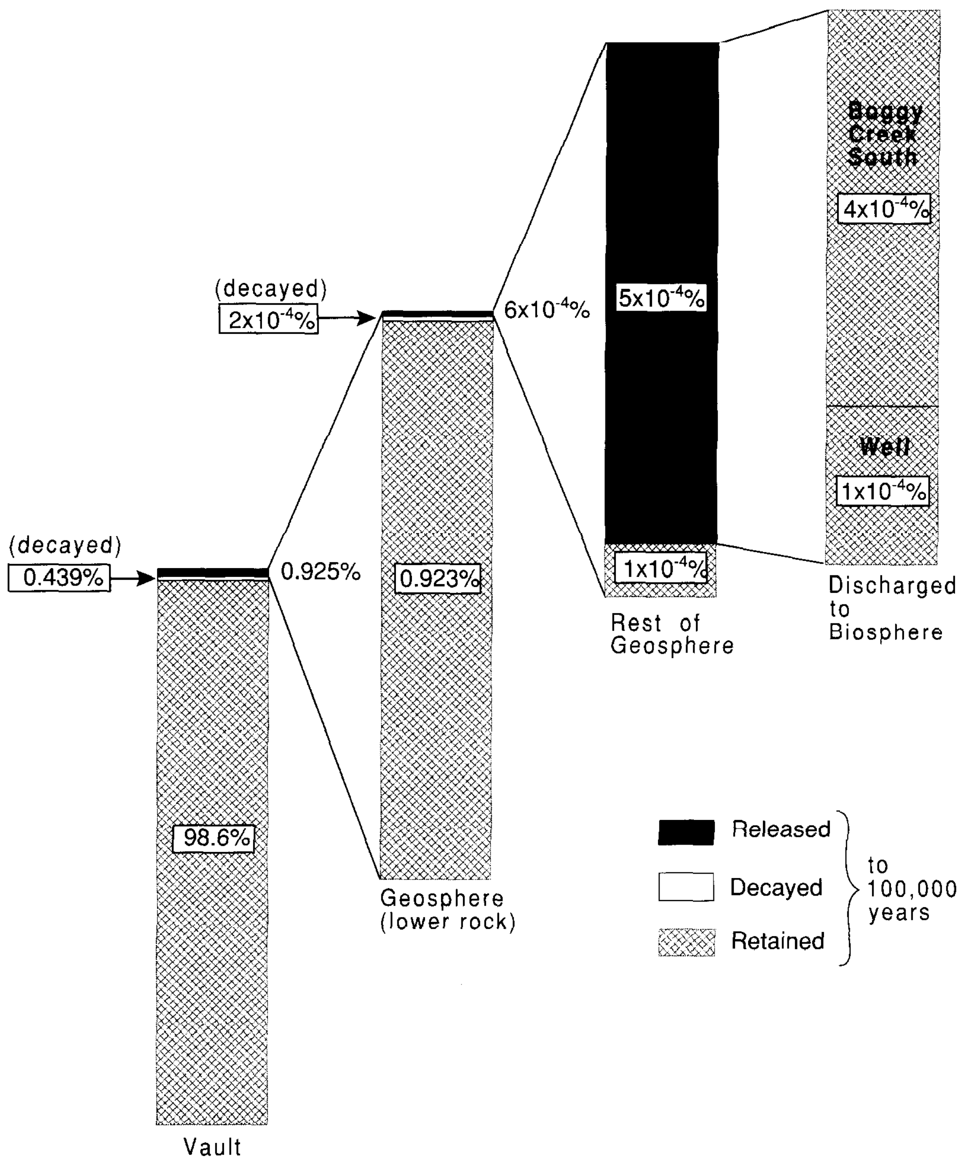

FIGURE D-23: Distribution of ^{129}I in the Geosphere after 10^5 a

All percentage values are relative to the initial inventory of ^{129}I (56 100 mol, or 7240 kg). A large percentage, 98.6% of the initial inventory of ^{129}I remains within the vault, and 0.925% reaches the lower rock zone after 10^5 a. Most of this 0.925% remains in the lower rock zone, with 6×10^{-4}% reaching the rest of the geosphere. Only 1×10^{-4}% is retained in the rest of the geosphere. After 10^5 a, a total of about 5×10^{-4}% (0.28 mol, or 36 g) has discharged to the well and Boggy Creek South in the biosphere. Radioactive decay has a minor effect.

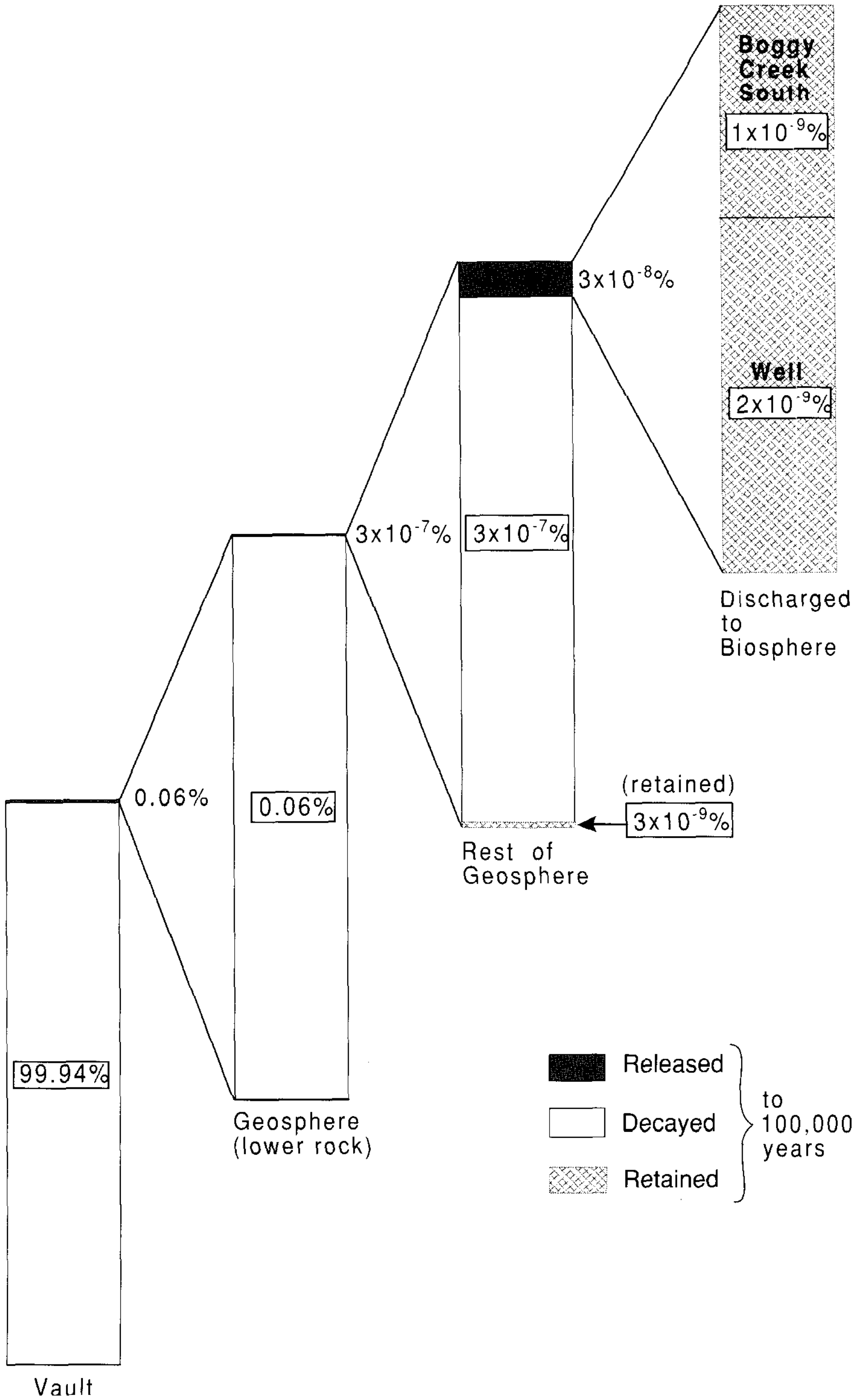

FIGURE D-24: Distribution of ^{14}C in the Geosphere after 10^5 a

All percentage values are expressed relative to the initial inventory of ^{14}C (2980 mol or 41.7 kg). Most of the ^{14}C decays (to stable N-14) before it can leave the vault and geosphere. For example, 99.94% of the initial inventory of ^{14}C decays within the vault, and only 0.06% reaches the lower rock zone after 10^5 a. Of this, only 3×10^{-7}% reaches the rest of the geosphere. An even smaller percentage reaches the biosphere: after 10^5 a, a total of about 3×10^{-8}% (9×10^{-7} mol, or 1×10^{-5} g) has discharged to the well and Boggy Creek South.

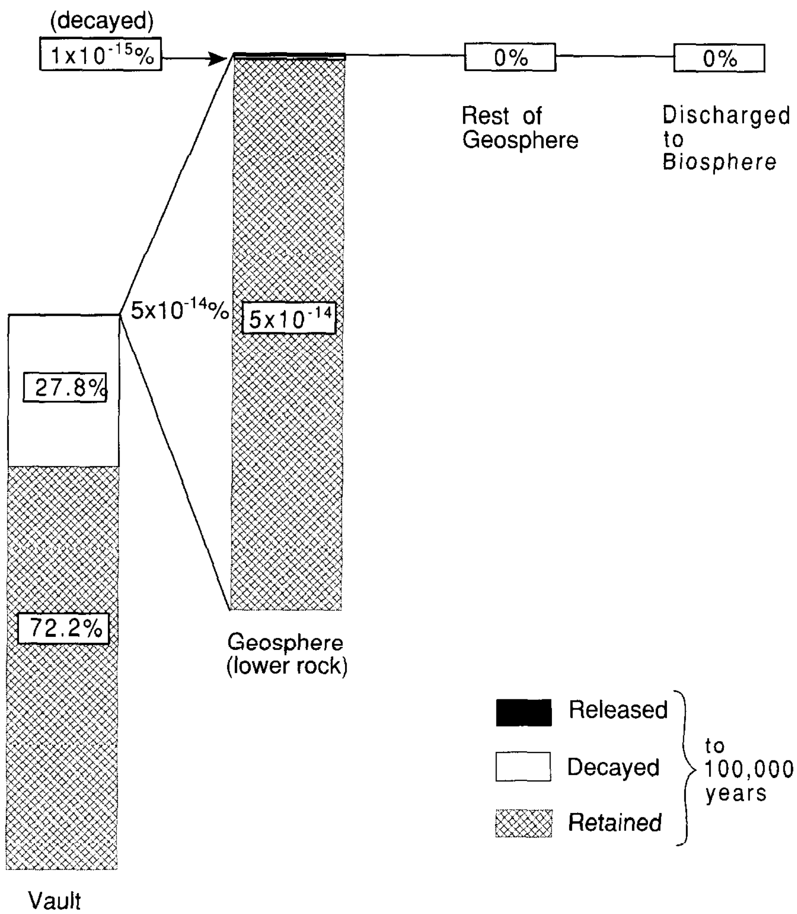

FIGURE D-25: Distribution of ^{99}Tc in the Geosphere after 10^5 a

All percentage values are expressed relative to the initial inventory of ^{99}Tc (335 000 mol, or 33 200 kg). No significant quantities of ^{99}Tc are found outside of the vault after 10^5 a. Within the vault, about 27.8% has decayed (to stable ^{99}Ru) and 72.2% is retained.

- Insignificant quantities, less than 5.2×10^{-14}% (2×10^{-10} mol, or 2×10^{-11} kg) have reached the geosphere;

- Essentially none has discharged into the biosphere, and

- The remainder of the ^{99}Tc inventory, about 28%, has undergone radioactive decay. Most of the decay occurs in the vault because little ^{99}Tc has escaped from the backfill.

Figure D-26 shows the distribution of ^{238}U in the disposal system after 10^5 a. Most of the ^{238}U remains in the vault; insignificant quantities have reached the lower rock zone, and none has reached the rest of the geosphere or the biosphere. Figure D-26 is representative of the distributions of many other contaminants. For example, the distributions of ^{234}U, ^{230}Th and ^{226}Ra are similar, in that no significant quantities are released from the lower rock zone in the geosphere and, therefore, there are no effects in the biosphere.

D.4 RESULTS FROM THE BIOSPHERE MODEL

In the following sections, we examine in detail the movement and fate of contaminants in the biosphere for the median-value simulation. We begin by describing the relevant characteristics of the critical group, and then describe the behaviour of ^{129}I and ^{14}C in the biosphere. Section 5.6 in the main text outlines the biosphere model, with more detail provided by Davis et al. (1993).

D.4.1 DESCRIPTION OF THE CRITICAL GROUP

As discussed in Chapters 2 and 5 of the main text, we assume that the critical group is a self-sufficient rural household, consisting of three adults in the median-value simulation. Their food includes produce from a garden, meat and dairy products from cattle and poultry raised on feed from a nearby forage field and fish caught in a nearby lake. They also eat wild berries, venison, upland birds and water fowl taken from their local surroundings.

Their garden is about 0.14 ha in size (one hectare equals 10^4 m^2) and lies on the terrestrial part of the discharge zone at Boggy Creek South (Figure D-27). We assume that the remainder of this terrestrial discharge zone is used for their forage field. An additional forage field is located on the terrestrial discharge zones at Boggy Creek North and Pinawa Channel. Their forage fields total about 9.2 ha, and parts lie outside of the dis charge zones. Their woodlot also lies outside of the discharge zones (Figure D-27).

Their dwelling is constructed of wood and bricks made from the local soil. The house is heated with wood from a nearby woodlot (there is no peat bog in the median-value simulation). The climate is comparable to present day conditions.

The household draws 1330 m^3/a from the well to supply all domestic water needs. Some of this water is also used for domesticated animals and for irrigating their garden.

D.4.2 CONTAMINANT RELEASE FROM THE GEOSPHERE TO THE BIOSPHERE

Contaminants from the vault pass through the geosphere and enter the biosphere pathways through groundwater sources. There are four locations where contaminated groundwater could enter the surface environment of the critical group: the well, and three low-lying discharge zones associated

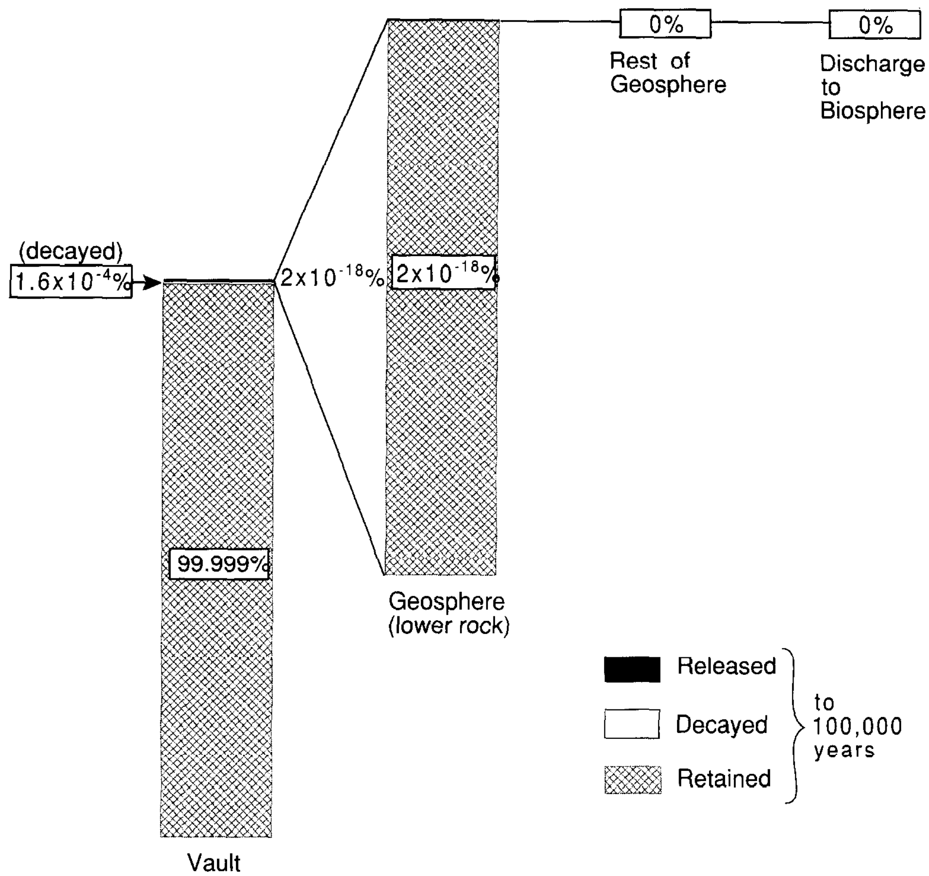

FIGURE D-26: Distribution of ^{238}U in the Geosphere after 10^5 a

All percentage values are relative to the initial inventory of ^{238}U (6.7×10^8 mol, or 1.6×10^8 kg). Essentially all of the ^{238}U is retained in the vault after 10^5 a, including a small amount (1.6×10^{-4}%) lost to radioactive decay. No significant quantities are found anywhere else in the disposal system, and no significant amounts are discharged to the biosphere.

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with a nearby body of surface water (Figure D-27). The total areas of these latter discharge zones are 29, 8 and 19 ha for Boggy Creek South, Boggy Creek North and Pinawa Channel respectively, and they receive 2200, 1200, and 500 m^3/a groundwater respectively. The terrestrial parts of these discharge zones are 1.6, 0.4 and 1.0 ha.

As discussed in Section D.3.2 (see, for example, Figure D-19), the largest discharges of contaminants for times up to 10^5 a occur at the well and Boggy Creek South, which are fed by fracture zone LD1. Moreover, the only radionuclides of concern are ^{129}I and ^{14}C from the used-fuel matrix. (Section D.3.3 notes that discharges of ^{14}C from used fuel into the biosphere

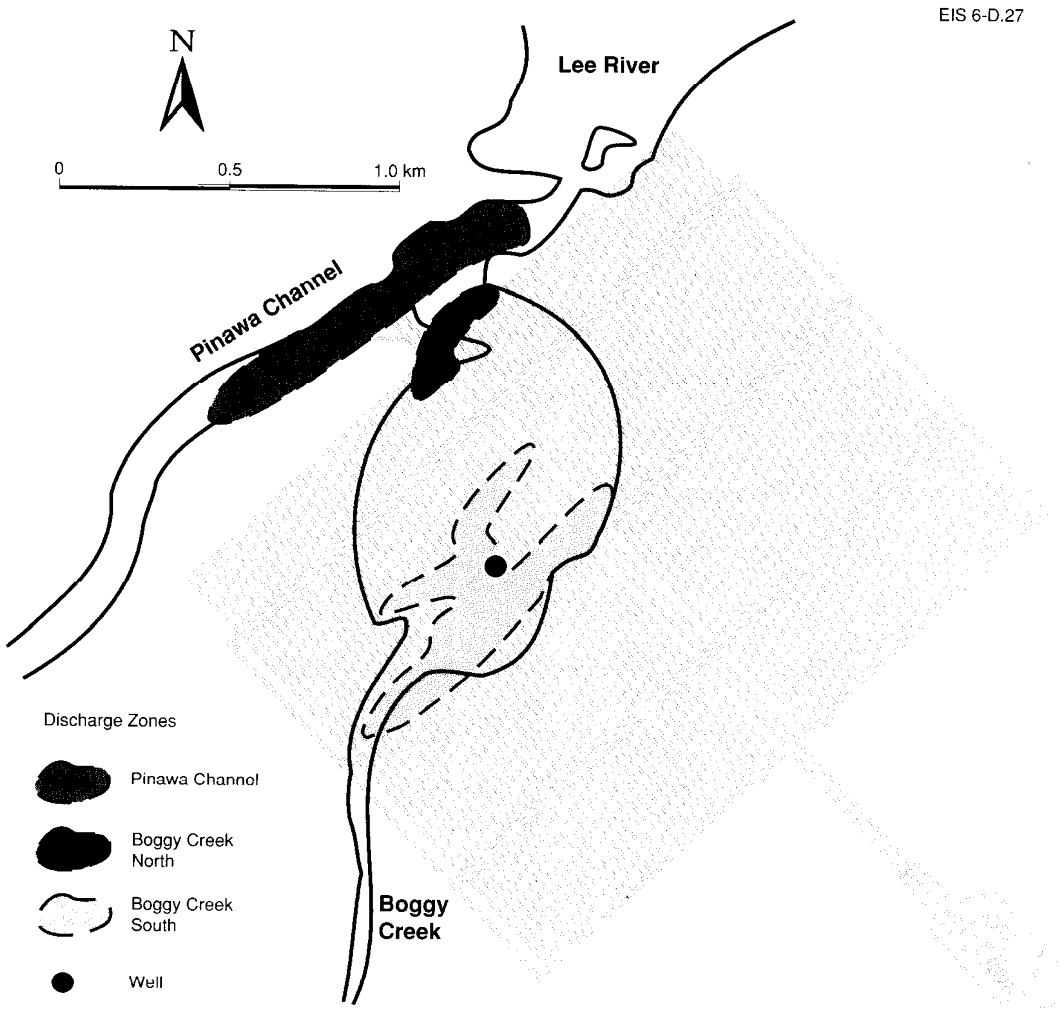

FIGURE D-27: Discharge Zones in the Biosphere

The system model for the reference disposal system assumes that contaminated groundwater from the vault passes through the geosphere and reaches the biosphere at four discharge zones: the well and three topographic lows (Boggy Creek South, Boggy Creek North and Pinawa Channel). However, for times up to 10^5 a in the median-value simulation, the only significant discharges are to the well and Boggy Creek South (Section D.3.3 of Appendix D). The biosphere model assumes that part of the discharge to the three topographic lows is to adjacent terrestrial zones and that the agricultural land used by the critical group overlies these terrestrial zones.

In the median-value simulation, the depth of the well is 37 m. It is located within the current confines of Boggy Creek because the geosphere model constrains the location of the well to lie along the centre of the contaminant plume that is moving up fracture zone LD1.

are overestimated, based on recent data (Johnson et al. 1994) for its instant-release fraction. Thus concentrations of ^{14}C and doses from ^{14}C reported herein are also overestimates. There are also discharges of ^{14}C from the Zircaloy matrix. However, its rates and total discharges are extremely small, and ^{14}C from the Zircaloy matrix is not discussed further.) The only chemically toxic contaminant with significant discharges is bromine.

The critical group uses 1330 m^3/a of water from the well in the median-value simulation, to supply all their domestic water needs. Included with this water are contaminants from the geosphere. The maximum annual discharge rates to the well at times up to 10^5 a are 3×10^{-6} mol/a of ^{129}I, 1×10^{-11} mol/a ^{14}C and 6×10^{-7} mol/a bromine. After 10^5 a, the total amounts discharged to the well are

- 0.074 mol (9.5 g) of ^{129}I,

- 5.1×10^{-7} mol (7.1×10^{-6} g) of ^{14}C and

- 1.4×10^{-2} mol (1.1 g) of bromine.

As indicated in Figure D-27, the garden and part of the forage field are located in the discharge zone at Boggy Creek South. Groundwater from this discharge zone also contains contaminants from the geosphere. The annual discharge rates to Boggy Creek South at 10^5 a are 9×10^{-6} mol/a ^{129}I, 2×10^{-12} mol/a ^{14}C and 6×10^{-7} mol/a bromine. After 10^5 a, the total amounts discharged to Boggy Creek South are

- 0.20 mol (26 g) of ^{129}I,

- 3.0×10^{-7} mol (4.2×10^{-6} g) of ^{14}C, and

- 9.8×10^{-2} mol (7.8 g) of bromine.

Figures D-28 and D-29 show the annual discharge rates for ^{129}I and ^{14}C. The curves show that

- Iodine-129 rates steadily rise over the period. They result in a maximum well water concentration of 2×10^{-9} mol/m^3 at 10^5 a. (If the calculations were extended further in time, the global maximum would occur after about 10^6 a.)

- Carbon-14 rates go through a maximum, partly because of the effects of radioactive decay. The maximum ^{14}C concentration in well water is 1×10^{-14} mol/m^3 near 5.5×10^4 a.

- Iodine-129 is discharged at a greater rate to Boggy Creek South than to the well because Boggy Creek South captures a larger portion of the contaminant plume.

- In contrast, ^{14}C is discharged at a larger rate to the well than to Boggy Creek South. It has a lower discharge rate to Boggy Creek South because of the additional transport time that is needed for the longer flow path leading to Boggy Creek South.

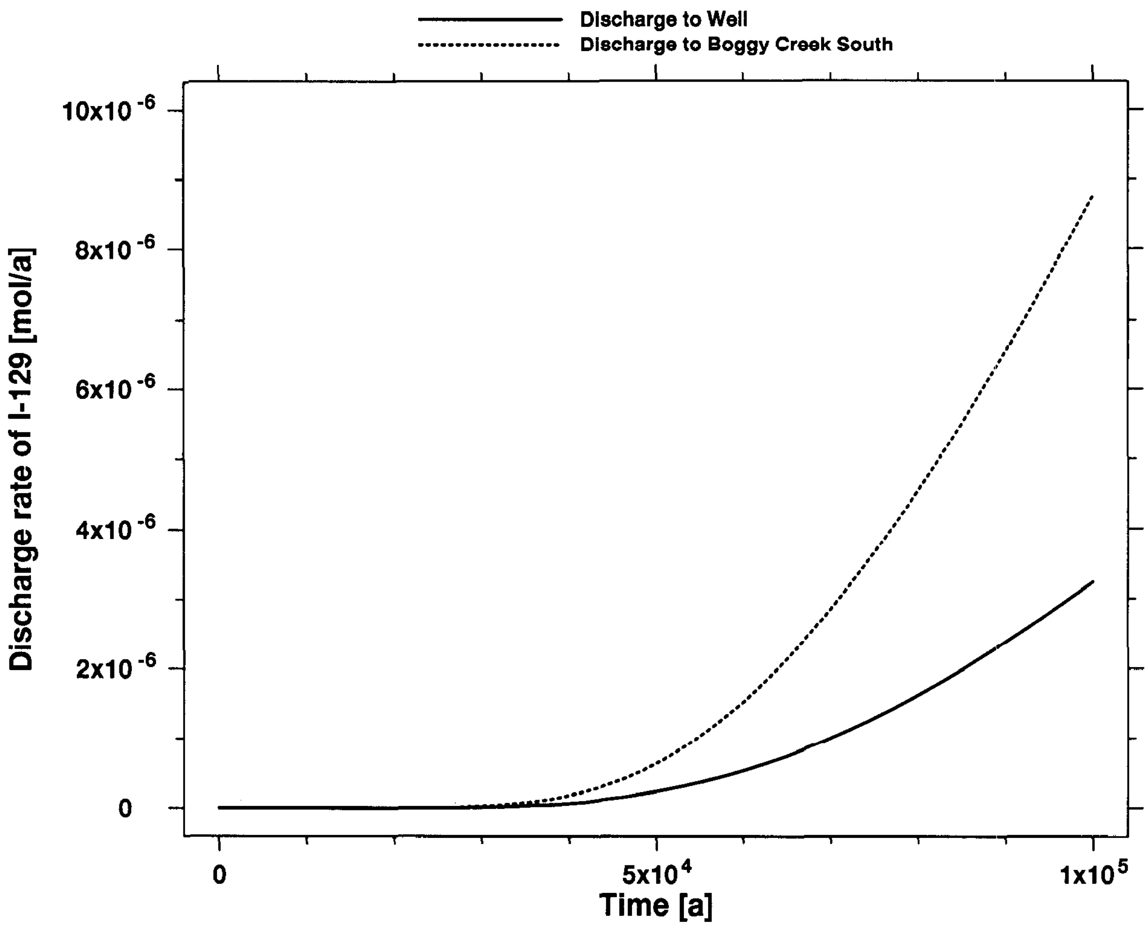

FIGURE D-28: Estimated ^{129}I Annual Discharge Rates to the Biosphere for the Median-Value Simulation

For times up to 10^5 a after vault closure, there are only two significant discharge zones to the biosphere: the well and Boggy Creek South. For ^{129}I, the annual discharge rates are extremely small up to about 3×10^4 a. The rates slowly increase and are still rising after 10^5 a. At that time, a total of about 0.27 mol (35 g) of ^{129}I has discharged to the biosphere.

This additional transport time is sufficient to decrease ^{14}C releases resulting from radioactive decay (it is not important for ^{129}I which has a much longer half-life). Carbon-14 release rates to Boggy Creek South reach a maximum of about 8×10^{-12} mol/a near 6.6×10^4 a.

D.4.3 IODINE-129 AND ^{14}C CONCENTRATIONS IN THE LAKE AND LAKE SEDIMENTS

In the median-value simulation, the lake (assumed to be the body of water called Boggy Creek in Figure D-27 (Davis et al. 1993)) covers 8 ha and is 5 m deep on average. Water enters the lake by inflow upstream, precipitation, runoff and upward flows of groundwater from the underlying rocks,

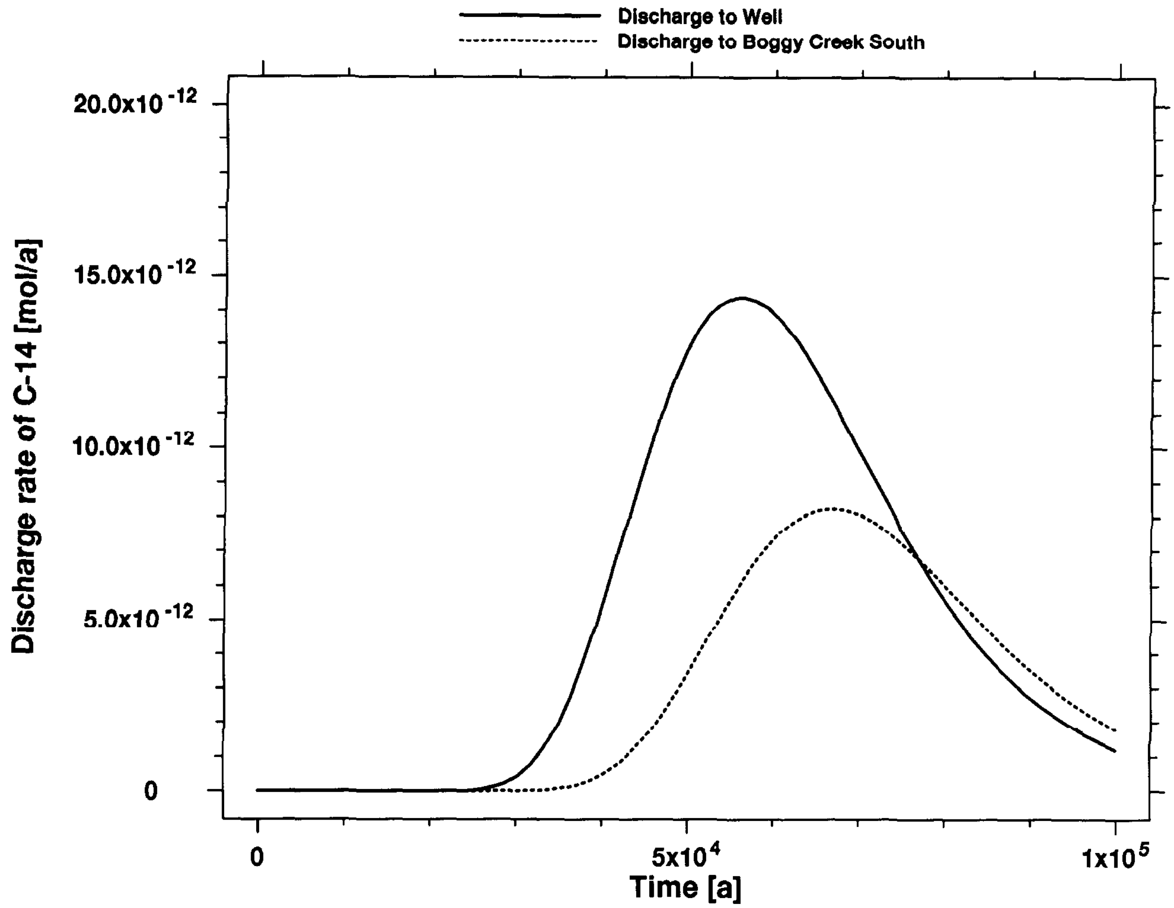

FIGURE D-29: Estimated ^{14}C Annual Discharge Rates to the Biosphere for the Median-Value Simulation

For times up to 10^5 a after vault closure, there are only two significant discharge zones to the biosphere: the well and Boggy Creek South. For ^{14}C, the annual discharge rates are extremely low up to about 3 x 10^4 a. The rates reach a maximum near 6 x 10^4 a, largely because of radioactive decay (the half-life of ^{14}C is 5730 a). After 10^5 a, a total of about 8.1 x 10^{-7} mol (1.1 x 10^{-5} g) of ^{14}C has discharged to the biosphere.

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then leaves the lake by outflow downstream. Each year 30 million cubic metres of runoff water (about 90 times the volume of the lake) pass through the lake.

As noted in Section 5.6 in the main text, we assume that all contaminants discharged to the biosphere enter the lake. Including all these discharges, the maximum contaminant concentrations calculated in the lake water are

- 4 x 10^{-13} mol/m^3 for ^{129}I, occurring at 10^5 a (the time cutoff of the simulations); and

- 6×10^{-19} mol/m^3 for ^{14}C, occurring near 6.0×10^4 a. (Section D.4.7 explains why maximum concentrations of ^{14}C in the well and in the lake occur at slightly different times.)

Concentrations in the lake water are much smaller than in the well water at any time because of dilution by the large volume of runoff water passing through the lake.

Concentrations are different in the two layers of lake sediment because these layers are contaminated from different sources:

- The lower layer of compacted sediment sorbs contaminants from the rising groundwater. The maximum concentrations in compacted sediment are 1×10^{-10} mol/kg for ^{129}I, occurring at 10^5 a, and 3×10^{-16} mol/kg for ^{14}C, occurring near 6.6×10^4 a.

- The upper layer of mixed sediment is contaminated as settling particles sorb contaminants from lake water. The maximum concentrations in mixed sediment are 1×10^{-12} mol/kg for ^{129}I, occurring at 10^5 a, and 2×10^{-18} mol/kg for ^{14}C, occurring at about 6.0×10^4 a.

D.4.4 IODINE-129 AND ^{14}C CONCENTRATIONS IN THE SOILS

In the median-value simulation, the soils in the garden, forage field and woodlot are sandy, with an average depth of 1.5 m above the water table. The soil model computes contaminant concentrations for the top two surface layers and a bottom layer for each of these fields. The surface layers together make up 0.3 m of rooting zone for plants. The bottom layer in the soil profile, 0.2 m thick, is in contact with the water table.

Figure D-27 shows the locations of the fields and discharge zones. Parts of the three discharge zones cover cultivatable land with areas amounting to 1.6, 0.4 and 1.0 ha for Boggy Creek South, Boggy Creek North and the Pinawa Channel respectively. The fields cultivated by the critical group are arranged on these land areas in such a fashion as to maximize the doses received through ingestion pathways:

- The 0.14-ha garden lies on the land part of the Boggy Creek South discharge zone that has the largest soil contaminant concentration of all the discharges at all times throughout the simulation period.

- The 9.2-ha forage field covers the remainder of the land area in the Boggy Creek South discharge, together with all of the land area in the Boggy Creek North and Pinawa Channel discharges, plus an additional area that is not over a discharge zone.

- The 9.5-ha woodlot lies entirely on land outside the discharge zones.

The garden, forage field and woodlot are just large enough to support the critical group household. Together, they are larger than the total land area associated with all three discharge zones, thus all the contaminants arriving at the surface can enter the food chain of the critical group.

Each type of field is contaminated by a different combination of three sources. Tables D-4 and D-5 list the ^{129}I and ^{14}C concentrations in the three fields, including

- The concentrations in the three sources of contamination (discharge of groundwater, irrigation using well water, and deposition from the atmosphere);

- The concentrations in the rooting zone of the soil with a breakdown by source; and

- The concentrations in the bottom layer of soil;

Figure D-30 summarizes the ^{129}I concentrations in the rooting zone and in the bottom soil layer in each field at 10^5 a. Figure D-31 shows the results for ^{14}C at 5.6×10^4 a. (Recent experimental data, discussed further in Section 8.2.6 in the main text, suggest that a smaller gaseous evasion rate from soil should be used for iodine and a larger rate, for carbon. These new data would lead to slightly larger concentrations in soil for ^{129}I and slightly smaller concentrations for ^{14}C.)

These tables and figures show that irrigation of the garden with well water causes the garden rooting zone to be much more contaminated than that of either the forage field or woodlot:

- The ^{129}I concentration in the garden soil reaches 2×10^{-10} mol/kg (soil) at 10^5 a, and

- The ^{14}C concentration reaches a maximum of 5×10^{-18} mol/kg (soil) near 5.6×10^4 a.

The ^{14}C concentration in the rooting zone of the soil is much lower relative to its concentration in the well water than is the case for ^{129}I, mostly because carbon degasses from soil 200 times faster than iodine. Hence the same concentrations in the source water would produce a relatively lower concentration of carbon than iodine in the soil.

The forage field and woodlot are contaminated primarily by deposition of gaseous ^{129}I released from the surface of the lake, a less efficient transport process than irrigation. The rooting zone of the soil in the forage field is slightly more contaminated with ^{129}I than in the woodlot. This is because the forage field lies partly over the Boggy Creek South discharge zone and, therefore, receives an additional influx of contaminants from discharging groundwater. The woodlot lies entirely on an area free from contamination by rising groundwater. Similar observations can also be made for ^{14}C, although its estimated concentrations in surface soils for the forage field and woodlot are less than 10^{-20} mol/kg (soil) and are reported as zero in Figure D-31.

In all three fields, discharging groundwater makes the smallest contribution to the rooting zone of the soil. The bottom layer of the forage field is more contaminated than the rooting zone for both ^{129}I and ^{14}C because the bottom layer is in direct contact with the groundwater at the water table.

TABLE D-4

ESTIMATED ^{129}I CONCENTRATIONS IN THE SOIL OF THE THREE FIELDS*

Concentration in	Garden	Forage Field	Woodlot
Rooting Zone of the Soil (mol/kg)			
- due to irrigation	2×10^{-10}	0	0
- due to deposition	2×10^{-13}	2×10^{-13}	2×10^{-13}
- due to groundwater	5×10^{-14}	8×10^{-15}	0
Total	2×10^{-10}	2×10^{-13}	2×10^{-13}
Bottom Soil (mol/kg)			
- due to groundwater	6×10^{-13}	1×10^{-13}	0
Source (mol/m^3)			
- irrigation water	2×10^{-9}	0	0
- deposition (air)	3×10^{-12}	3×10^{-12}	3×10^{-12}
- groundwater	3×10^{-8}	4×10^{-9}	0

* These results are from the median-value simulation at 10^5 a after vault closure when ^{129}I concentrations are highest. The upper part of the table gives the estimated concentrations of ^{129}I in the rooting zone and bottom layer of the garden, forage field and woodlot. The sources of the ^{129}I are groundwater discharge, irrigation from the well and deposition from the atmosphere. The lower third of the table lists ^{129}I concentrations in these sources. A value of zero is reported for calculated concentrations less than 10^{-20} mol/kg dry soil.

D.4.5 IODINE-129 AND ^{14}C CONCENTRATIONS IN THE ATMOSPHERE

Contaminants in water and soil can enter the air above them by processes that include wind or mechanical dust suspension, degassing, burning of vegetation to clear land and to heat dwellings, forest fires, spraying water to irrigate land and spraying of water indoors by showers and humidifiers.

Tables D-6 and D-7 show the contributions by various routes to indoor and outdoor air concentrations of ^{129}I and ^{14}C. The maximum estimated indoor air concentrations are

- 2×10^{-14} mol/m^3 for ^{129}I, occurring at 10^5 a; and
- 1×10^{-19} mol/m^3 for ^{14}C, occurring near 5.6×10^4 a.

For both nuclides, 90% of the contribution to inside air is from spraying in showers and humidifiers; most of the remainder is from degassing garden soil.

TABLE D-5

ESTIMATED ^{14}C CONCENTRATIONS IN THE SOIL OF THE THREE FIELDS*

Concentration in	Garden	Forage Field	Woodlot
Rooting Zone of the Soil (mol/kg)			
- due to irrigation	5×10^{-18}	0	0
- due to deposition	0	0	0
- due to groundwater	0	0	0
Total	5×10^{-18}	0	0
Bottom Soil (mol/kg)			
- due to groundwater	4×10^{-18}	6×10^{-19}	0
Source Water (mol/m^3)			
- irrigation	1×10^{-14}	0	0
- deposition	1×10^{-18}	1×10^{-18}	1×10^{-18}
- groundwater	3×10^{-15}	4×10^{-16}	0

* These results are from the median-value simulation at 5.6×10^4 a after vault closure when the estimated annual dose from ^{14}C is greatest. The upper part of the table gives the estimated concentrations of ^{14}C in the rooting zone and bottom layer of the garden, forage field and woodlot. The sources of the ^{14}C are groundwater discharge, irrigation from the well and deposition from the atmosphere. The lower third of the table lists ^{14}C concentrations in these sources. A value of zero is reported for calculated concentrations less than 10^{-20} mol/kg dry soil.

The maximum estimated outdoor air concentrations are

- 1×10^{-15} mol/m^3 for ^{129}I, occurring at 10^5 a; and
- 1×10^{-20} mol/m^3 for ^{14}C, occurring near 5.6×10^4 a.

In both cases, 99% is due to degassing from garden soil. (Recent experimental data, discussed further in Section 8.2.6 in the main text, would revise the gaseous evasion rates from soil for iodine and for carbon. The new data would lead to slightly lower concentrations in indoor and outdoor air for ^{129}I, and slightly higher concentrations for ^{14}C.)

D.4.6 ANNUAL DOSE ESTIMATES FROM ^{129}I AND ^{14}C

The biosphere model describes 23 exposure pathways, accounting for contaminates in the following sources:

- drinking water from the well or lake;

- garden plants contaminated via roots, and via leaves;

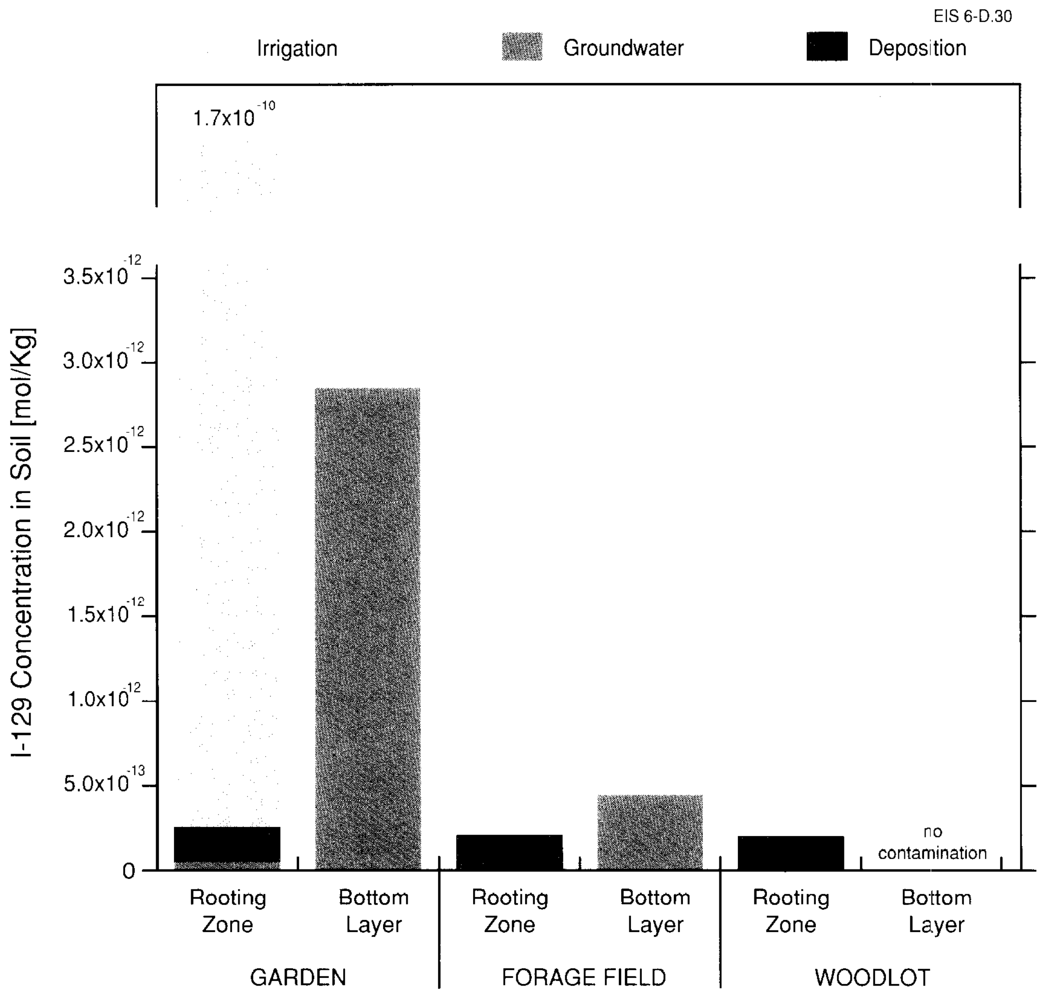

FIGURE D-30: Estimated ^{129}I Concentrations in the Rooting Zone and Bottom Layer of the Soils at 10^5 a

This histogram shows ^{129}I concentrations from the median-value simulation along the vertical axis. The horizontal axis identifies the soil layers (rooting zone and bottom layer) of the three fields (garden, forage field and woodlot). Contributions for the sources of the contamination (groundwater discharge, irrigation and atmospheric deposition) are also indicated.
The rooting zone of the garden has the largest ^{129}I concentration, primarily because of irrigation of the garden with well water. The bottom soil of the garden has a much lower concentration, whose source is groundwater discharge. The forage field soils have much lower concentrations, arising from groundwater discharge and deposition. The woodlot soils are contaminated by deposition only because the woodlot is not within a groundwater discharge zone. Thus the bottom soil of the woodlot is not contaminated.

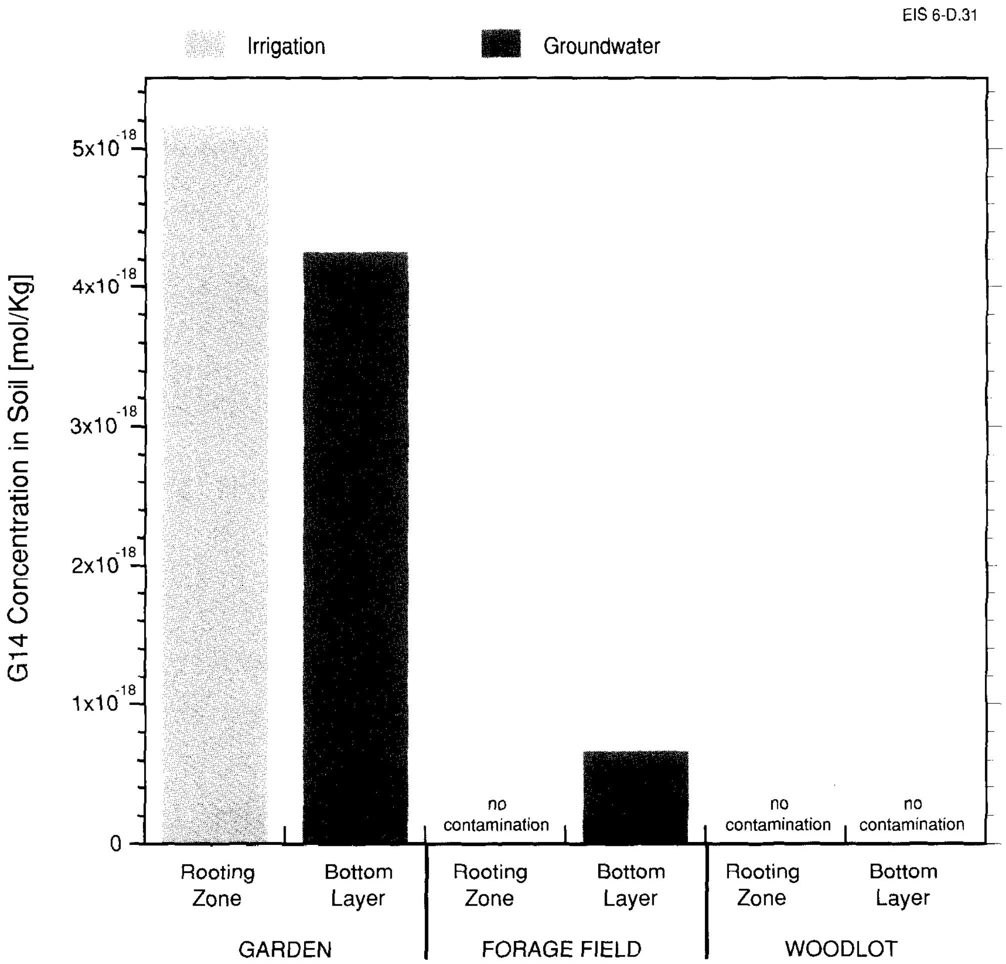

FIGURE D-31: Estimated ^{14}C Concentrations in the Rooting Zone and Bottom Layer of the Soils at 5.6×10^4 a

This histogram shows ^{14}C concentrations from the median-value simulation along the vertical axis. The horizontal axis identifies the soil layers (rooting zone and bottom layer) of the three fields (garden, forage field and woodlot). Contributions for the sources of the contamination (groundwater discharge, irrigation and atmospheric deposition) are also indicated.

The rooting zone of the garden has the highest ^{14}C concentration, primarily due to irrigation of the garden with well water. Groundwater discharge and atmospheric deposition both contribute less than 10^{-20} mol/kg (soil). The bottom soil of the garden has the next highest concentration, resulting from groundwater discharge. The only other nonzero concentration is the bottom soil of the forage field, also resulting from groundwater discharge. The other concentrations are reported as zero; the estimated concentrations are much less than 10^{-20} mol/kg. These estimated concentrations show small contributions from groundwater discharge and atmospheric deposition for the surface soil of the forage field, and from atmospheric deposition only for the surface soil of the woodlot.

TABLE D-6

ESTIMATED ^{129}I CONCENTRATIONS IN AIR*

Source	Contribution to indoor air (mol/m^3)	Contribution to outdoor air (mol/m^3)
Showers and humidifiers	2×10^{-14}	0
Gas released from garden soil	1×10^{-15}	1×10^{-15}
Suspended particles from garden soil	1×10^{-17}	1×10^{-17}
Gas released from surface of lake	5×10^{-18}	5×10^{-18}
Wood burning to heat dwelling	0	4×10^{-20}
Stubble burning	0	0
Land clearing fires and forest fires	0	0
Suspended particles from the lake	0	0
Total:	2×10^{-14}	1×10^{-15}

* These results are from the median-value simulation at 10^5 a after vault closure when ^{129}I concentrations are highest. The largest ^{129}I contribution to indoor air is from showers and humidifiers; for outdoor air it is degassing from garden soil. A value of zero is reported for calculated concentrations less than 10^{-20} mol/m^3.

TABLE D-7

ESTIMATED ^{14}C CONCENTRATIONS IN AIR*

Source	Contribution to Indoor Air (mol/m^3)	Contribution to Outdoor Air (mol/m^3)
Showers and humidifiers	1×10^{-19}	0
Gas released from garden soil	1×10^{-20}	1×10^{-20}
Suspended particles from garden soil	0	0
Gas released from surface of lake	0	0
Wood burning to heat dwelling	0	0
Stubble burning	0	0
Land clearing fires and forest fires	0	0
Suspended particles from the lake	0	0
Total:	1×10^{-19}	1×10^{-20}

* These results are from the median-value simulation at 5.6×10^4 a after vault closure, when estimated annual dose from ^{14}C is largest. The largest ^{14}C contribution to indoor air is from showers and humidifiers; for outdoor air it is degassing from garden soil. A value of zero is reported for calculated concentrations less than 10^{-20} mol/m^3.

- meat, poultry and dairy products contaminated by drinking water, soil, or feed contaminated via roots and via leaves of plants in the forage field;

- fish contaminated by the lake water; and

- soil directly ingested with food and contaminated, as described earlier.

The dominant pathway for radiation doses is ingestion of contaminants in the food-chain. Impacts are also estimated for other pathways: inhalation, and external exposure to contaminated soil, water, air, and organic and inorganic building materials.

Figures D-32 and D-33 illustrate the contributions to the maximum annual dose estimates (ADE) from ^{129}I and ^{14}C from the more important pathways in the median-value simulation. A more detailed breakdown is summarized in Tables D-8 and D-9.

Over 99% of the ^{129}I ADE is internal and is incurred through pathways to man starting at the well. At 10^5 a after vault closure, the time of the maximum ADE from ^{129}I

- Consumption of garden plants contaminated through their roots and leaves contributes about 37% and 28% of the maximum ADE. Over 99% of the contamination of both roots and leaves originates in the well water used to irrigate the garden.

- About 23% of the maximum ADE is due to drinking contaminated well water.

- Consumption of meat, poultry and dairy products contaminated through the animals' drinking water contribute about 2%, 2% and 4% respectively to the maximum ADE.

- Inhalation of contaminated air contributes about 2%.

Most of the maximum ADEs from ^{14}C are also from internal pathways and start at the well. The ADEs from ^{14}C reach a maximum near 5.6 x 10^4 a after closure; at longer times its radioactive decay results in smaller doses.

At this time (compare also Figure D-33 and Table D-9)

- About 55% of the maximum ADE attributed to ^{14}C comes from consuming garden plants;

- About 22% from drinking well water;

- About 12%, 5%, and 5% from consuming meat, milk and poultry products respectively, contaminated through animals' drinking water; and

- About 1% from consuming fish (Figure D-33).

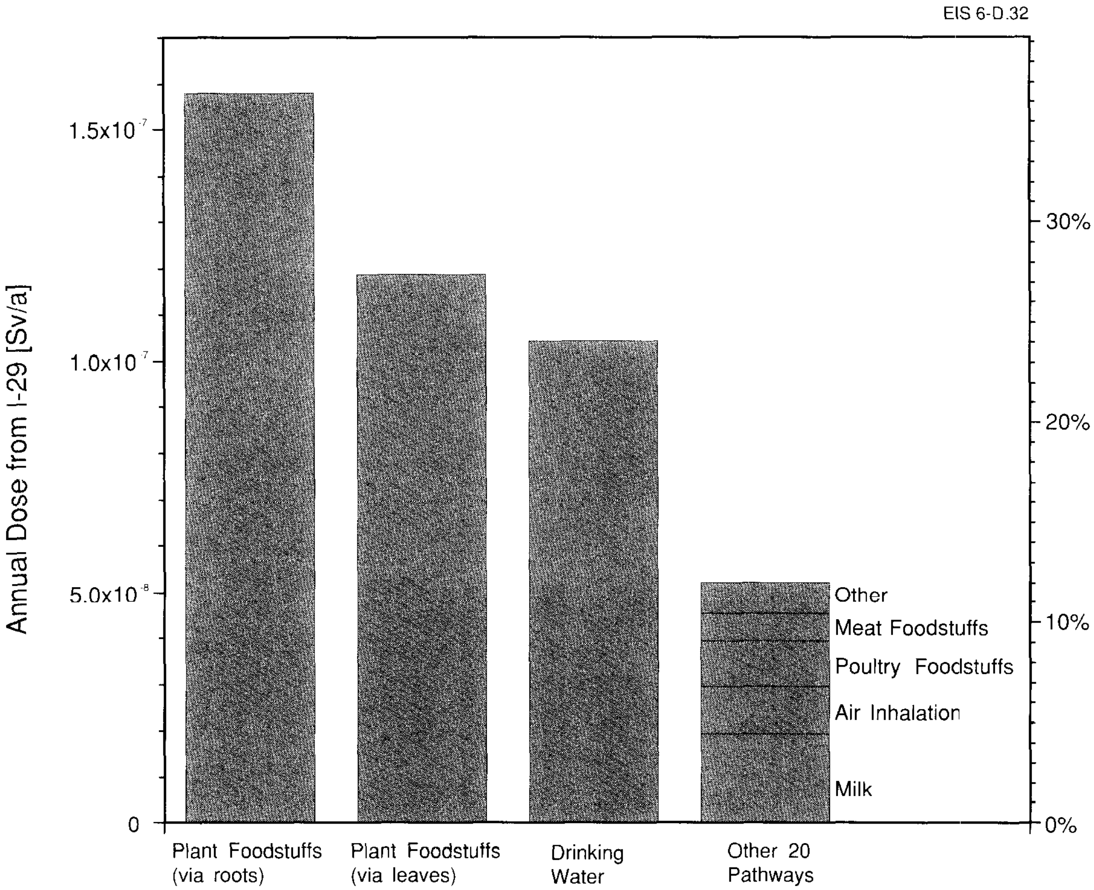

FIGURE D-32: Contributions by Pathway of Annual Doses from ^{129}I

These results, from the median-value simulation, show the breakdown by pathway of the annual dose from ^{129}I at 10^5 a. The total annual dose, about 4.3×10^{-7} Sv/a, is dominated by internal pathways, particularly ingestion of garden plants and drinking water.

For all but the fish pathway, the main source of ^{14}C is well water. The breakdown of the ^{14}C ADEs from the various pathways differs from that for ^{129}I because of the different degrees with which the two nuclides move from soil to plant, from plant to animal, and from water to fish.

For both ^{129}I and ^{14}C, ingestion pathways tend to give larger ADEs than inhalation, and these internal pathways dominate external doses. Ingestion doses from plant foods are greater than from drinking well water because contaminants accumulate in garden soil irrigated with well water and in the plants grown on them. In contrast, animals are more contaminated by the well water they drink than by their feed. The feed comes from an unirrigated forage field that lies over less contaminated discharge areas than the garden.

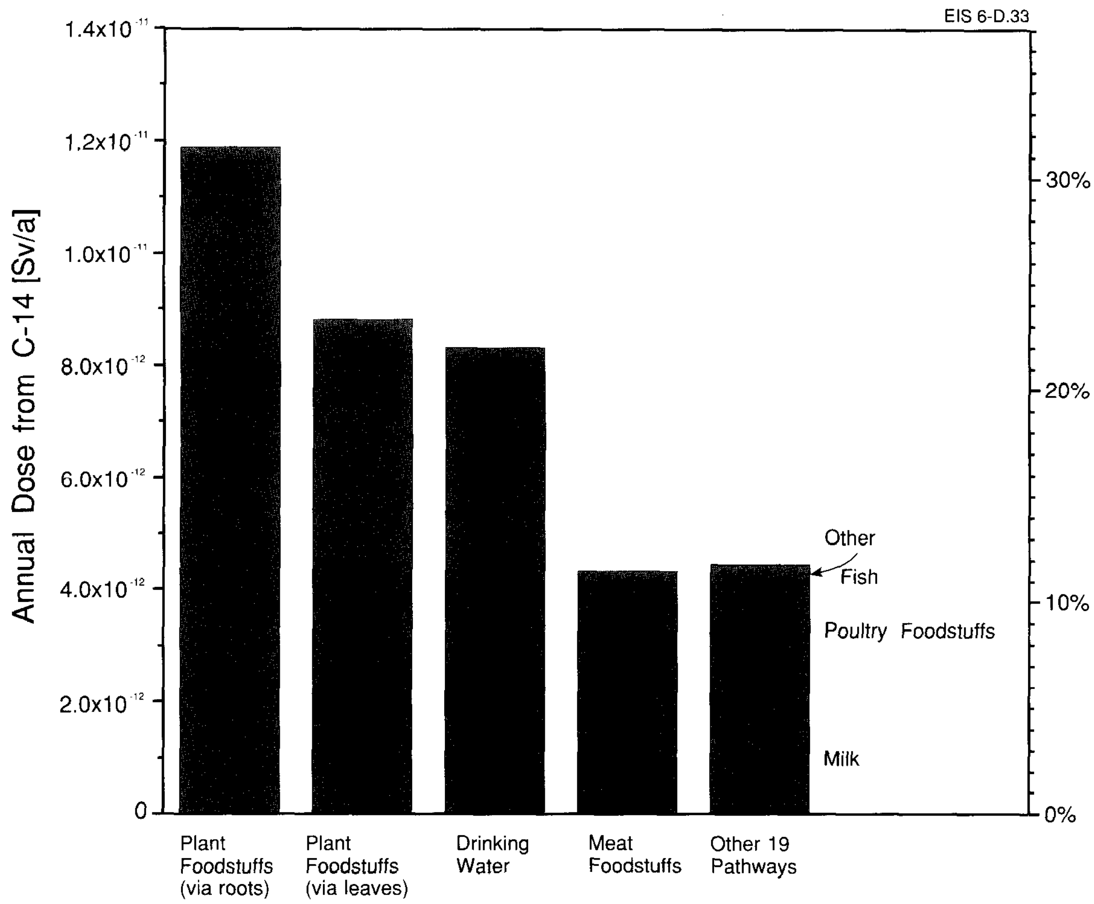

FIGURE D-33: Contributions by Pathway of Annual Doses from ^{14}C

These results, from the median-value simulation, show the breakdown by pathway of the annual dose from ^{14}C at 5.6 x 10^4 a. The total annual dose, about 3.8 x 10^{-11} Sv/a, is dominated by internal pathways, particularly ingestion of garden plants, drinking water and animal products.

Movement of ^{129}I in gaseous form dominates transport between some parts of the biosphere. As mentioned above, the soils of the forage field and woodlot are contaminated by deposition of ^{129}I released from the lake surface by gaseous evasion. Concentrations of ^{129}I in outdoor air are controlled largely by degassing from garden soil; concentration in indoor air arises mostly from release of gaseous ^{129}I from water used in showers and humidifiers. However, in each case the affected pathways to man are less important than more direct ingestion pathways starting with ^{129}I in well water.

TABLE D-8

BREAKDOWN OF ESTIMATED ANNUAL DOSES FROM ^{129}I*

Pathway (and source)	Dose to man (Sv/a)
Ingestion Pathways	
- water (well water)	1.0×10^{-7}
- garden and other plants	
root uptake from soil	1.6×10^{-7}
leaf uptake from irrigation water and air	1.2×10^{-7}
- dairy products	
well water	1.9×10^{-8}
feed-leaf uptake from air	2.5×10^{-9}
feed-root uptake from soil	6.2×10^{-11}
feed-ingested soil	2.7×10^{-11}
- poultry products (including wild birds)	
well water	9.7×10^{-9}
feed-leaf uptake from air	8.7×10^{-10}
feed-root uptake from soil	3.1×10^{-11}
feed-ingested soil	1.2×10^{-11}
- mammalian meat products (wild and domesticated)	
well water	6.0×10^{-9}
feed-leaf uptake from air	7.6×10^{-10}
feed-root uptake from soil	2.4×10^{-11}
feed-ingested soil	1.0×10^{-11}
- fish from the lake	1.2×10^{-11}
- soil from the garden (directly ingested)	2.5×10^{-9}
Inhalation	
- showers and humidifiers, gas from garden soil	1.0×10^{-8}
Total for internal pathways (ingestion plus inhalation):	4.3×10^{-7}
External Dose	
- ground exposure (garden)	5.8×10^{-11}
- inorganic building materials (woodlot, soil)	1.4×10^{-11}
- water immersion (well water)	1.1×10^{-12}
- air immersion (showers, humidifiers, gas from garden soil)	2.0×10^{-13}
Total for external pathways:	7.3×10^{-11}
Total for internal and external pathways:	4.3×10^{-7}

* The results give a breakdown of the pathways and sources for estimated annual doses from ^{129}I for the median-value simulation. The values are given at 10^5 a, where estimated annual doses from ^{129}I have reached a maximum for the simulation.

TABLE D-9

BREAKDOWN OF ESTIMATED ANNUAL DOSES FROM ^{14}C*

Pathway (and source)	Dose to man (Sv/a)
Ingestion Pathways	
- water (well water)	8.3×10^{-12}
- garden and other plants	
root and leaf uptake from soil, irrigation water and air	2.1×10^{-11}
- dairy products	
well water	2.3×10^{-12}
feed-root and leaf uptake	6.6×10^{-16}
feed-ingested soil	2.2×10^{-18}
- poultry products (including wild birds)	
well water	1.8×10^{-12}
feed-root and leaf uptake	5.0×10^{-16}
feed-ingested soil	1.5×10^{-18}
- mammalian meat products (wild and domesticated)	
well water	4.4×10^{-12}
feed-root and leaf uptake	1.6×10^{-15}
feed-ingested soil	4.8×10^{-18}
- fish from the lake	3.6×10^{-13}
- soil from the garden (directly ingested)	1.4×10^{-15}
Inhalation	
- showers and humidifiers, gas from garden soil	8.8×10^{-15}
Total for internal pathways (ingestion plus inhalation):	3.8×10^{-11}
External Dose	
- ground exposure (garden soil)	5.2×10^{-19}
- dwelling construction materials (woodlot, soil)	0.0
- water immersion (well water)	3.3×10^{-17}
- air immersion (showers, humidifiers, gas from garden soil)	1.2×10^{-17}
Total for external pathways:	4.5×10^{-17}
Total for internal and external pathways:	3.8×10^{-11}

* The results give a breakdown of the pathways and sources for estimated annual doses from ^{14}C for the median-value simulation. The values are given at 5.6×10^4 a; at this time, the estimated annual dose from ^{14}C has reached a maximum for most pathways.

D.4.7 SUMMARY OF CONTAMINANT BEHAVIOUR IN THE BIOSPHERE

Over the 10^5 a following vault closure, the geosphere releases into the biosphere about

- 0.27 mol (35 g) of ^{129}I,
- 8.1×10^{-7} mol (1.1×10^{-5} g) of ^{14}C, and
- 0.11 mol (8.9 g) of bromine.

The releases of all other radionuclides and chemically toxic elements are negligible.

These small or negligible releases suggest that there would be no significant chemical toxicity or radiation doses from any of the contaminants in the nuclear fuel waste:

- Estimated concentrations of bromine are less than 3×10^{-10} mol/kg soil, 5×10^{-10} mol/m^3 water and 2×10^{-17} mol/m^3 air. These concentrations are many orders of magnitude below existing concentrations of bromine in the environment. Thus the additional contribution of bromine from the waste disposal facility would be negligible.

- The total ADE from all nuclides in the median-case simulation is almost entirely due to ^{129}I from the used-fuel matrix. The greatest value reached, at 10^5 a, is 4×10^{-7} Sv/a (Figures 6-2 and 6-3). This value amounts to less than 0.02% in the average annual dose from environmental radioactivity (about 3×10^{-3} Sv/a) received by individuals living today on the Canadian Shield. It is also less than 1% of the annual dose of 5×10^{-5} Sv/a associated with the AECB risk (AECB 1987).

Tables D-10 and D-11 summarize the estimated concentrations of ^{129}I and ^{14}C in different parts of the biosphere. No significant concentrations of any other radionuclides or chemically toxic contaminants exist within the biosphere. Transport out of the modelled system is through lake outflow and atmospheric dispersion; the subsequent highly diluted concentrations of contaminants are expected to have much smaller impacts than the estimated impacts to members of the critical group.

At 10^5 a following vault closure, over 97% of the ^{129}I discharged to the biosphere has left that portion of the biosphere that is modelled in the system model. The bulk of the 3% remaining in the local environment is in the sediments of the lake. Less than 0.1% remains in the field soils. Figure D-34 shows the net flows of ^{129}I in and out of the modelled part of the biosphere as a function of time.

Similarly by about 6.8×10^4 a, the time of maximum mass of ^{14}C in the biosphere, 95% of the ^{14}C discharged into the biosphere has left via the lake outflow. About 4% remains in lake sediment and 0.01% in field soils. Figure D-35 summarizes the net flows of ^{14}C in and out the modelled part of

TABLE D-10

CONCENTRATIONS OF ^{129}I IN THE BIOSPHERE*

Affected Part of Biosphere	^{129}I Concentration at 10^5a	Origin of Contamination
Well water	2×10^{-09} mol/m^3	Well
Lake water	4×10^{-13} mol/m^3	Well, Boggy Creek South
Garden soil	2×10^{-10} mol/kg	Irrigation with well water
Forage field soil	2×10^{-13} mol/kg	Degassing from the lake
Woodlot soil	2×10^{-13} mol/kg	Degassing from the lake
Lake sediment		
- compacted	1×10^{-10} mol/kg	Boggy Creek South
- mixed	2×10^{-11} mol/kg	Deposition from lake water
Garden plants	1×10^{-11} mol/kg	Root uptake from garden soil
Meat	8×10^{-13} mol/kg	Ingested well water
Milk	2×10^{-12} mol/m^3	Ingested well water
Poultry	3×10^{-12} mol/kg	Ingested well water
Fish	2×10^{-14} mol/kg	Lake water
Indoor air	2×10^{-14} mol/m^3	Showers and humidifiers
Outdoor air	1×10^{-15} mol/m^3	Degassing from garden soil

* These results, from the median-value simulation, show the estimated concentrations of ^{129}I in different parts of the biosphere at 10^5 a following vault closure. The last column indicates the origin of the ^{129}I.

the biosphere as a function of time. Note that, by 6.8×10^4 a, more than 99.9% of the initial inventory of ^{14}C in the disposal system has decayed to the stable nuclide, ^{14}N.

Concentrations of ^{14}C in different parts of the biosphere peak at slightly different times. For instance, concentrations in well water peak at 5.6×10^4 a, as do concentrations in parts of the biosphere that are mostly affected by well water (such as garden plants). Concentrations in lake water peak at a later time because lake concentrations slowly build up with time and because of the delayed arrival of additional discharges from the geosphere to Boggy Creek South. Forage field and woodlot soils peak at the same time as the lake water because the main contamination process is rapid deposition on these fields of ^{14}C released from the lake by gaseous evasion.

TABLE D-11

CONCENTRATIONS OF ^{14}C IN THE BIOSPHERE*

Affected Part of Biosphere	Peak ^{14}C Concentration	Time of Peak (a)	Origin of Contamination
Well water	1×10^{-14} mol/m^3	5.6×10^4	Well
Lake water	6×10^{-19} mol/m^3	6.0×10^4	Well, Boggy Creek South
Garden soil	5×10^{-18} mol/kg	5.6×10^4	Irrigation with well water
Forage field	0	6.0×10^4	Degassing from the lake
Woodlot soil	0	6.0×10^4	Degassing from the lake
Lake Sediment			
- deep	3×10^{-16} mol/kg	6.6×10^4	Boggy Creek South
- shallow	2×10^{-18} mol/kg	6.0×10^4	Deposition from lake water
Garden plants	5×10^{-17} mol/kg	5.6×10^4	Irrigation with well water
Meat	3×10^{-17} mol/kg	5.6×10^4	Ingested well water
Milk	1×10^{-17} mol/m^3	5.6×10^4	Ingested well water
Poultry	3×10^{-17} mol/kg	5.6×10^4	Ingested well water
Fish	3×10^{-17} mol/kg	6.0×10^4	Lake water
Indoor air	1×10^{-19} mol/m^3	5.6×10^4	Showers and humidifiers
Outdoor air	1×10^{-20} mol/m^3	5.6×10^4	Degassing from garden soil

* These results, from the median-value simulation, show the estimated concentrations of ^{14}C in different parts of the biosphere at times near 6.0×10^4 a following vault closure. The actual time chosen for each concentration is when the concentration has reached its maximum value. The last column indicates the origin of the ^{14}C. A value of zero is reported for calculated concentrations less than 10^{-20} mol/m^3 or mol/kg.

D.5 METHOD OF SENSITIVITY ANALYSIS

D.5.1 INTRODUCTION

Sensitivity analysis is used to improve our understanding of the operation of the system model. We outline in this section the systematic approach used for the median-value simulation.

It is convenient to distinguish two steps:

- First, we screen the parameters of the system model to identify important parameters. An important parameter is one that causes significant changes to some objective function when its value is

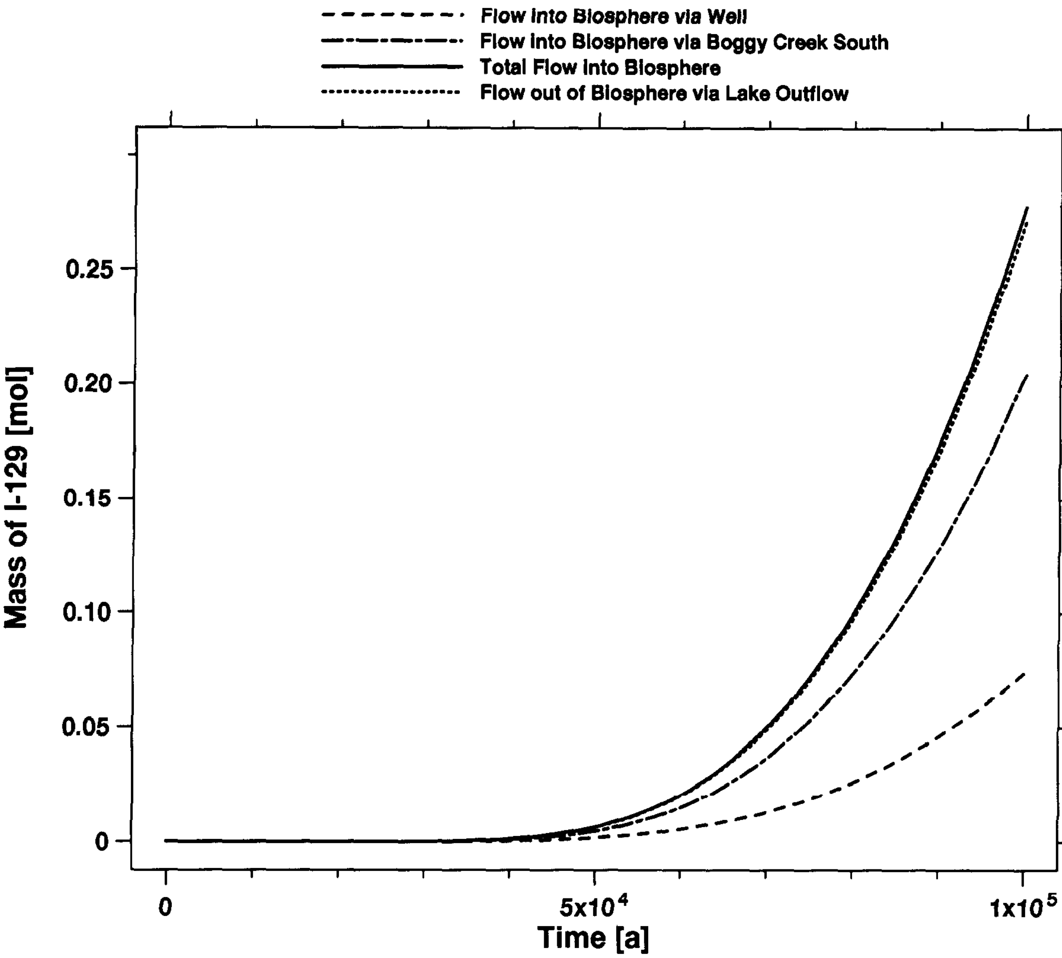

FIGURE D-34: Flows of ^{129}I in and out of the Modelled Biosphere

These curves show the ^{129}I flow in the modelled part of the biosphere for the median-value simulation. The topmost curve shows the total flow in; it is the sum of the bottom two curves, which represent flows in from Boggy Creek South and the well. The curve second from the top shows the total flow of ^{129}I out of the modelled portion of the biosphere, resulting from outflow in lake water.

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changed. Section D.5.2 describes the objective functions of interest. The main results of the screening for the median-value simulation are reported in the main text (Section 6.3.3). Additional results (using different objective functions) are discussed in Sections D.6 to D.8.

- Second, for each important parameter, we then show how it affects the results and investigate the reasons for these effects. These studies are documented in Sections D.6 to D.8.

One important use of sensitivity analysis of the median-value simulation is that it guides us in interpreting the results of the thousands of randomly sampled simulations, including the associated sensitivity analyses. Our experience has shown that systematic sensitivity analysis of the median-value simulation reveals many subtle effects and interactions that are

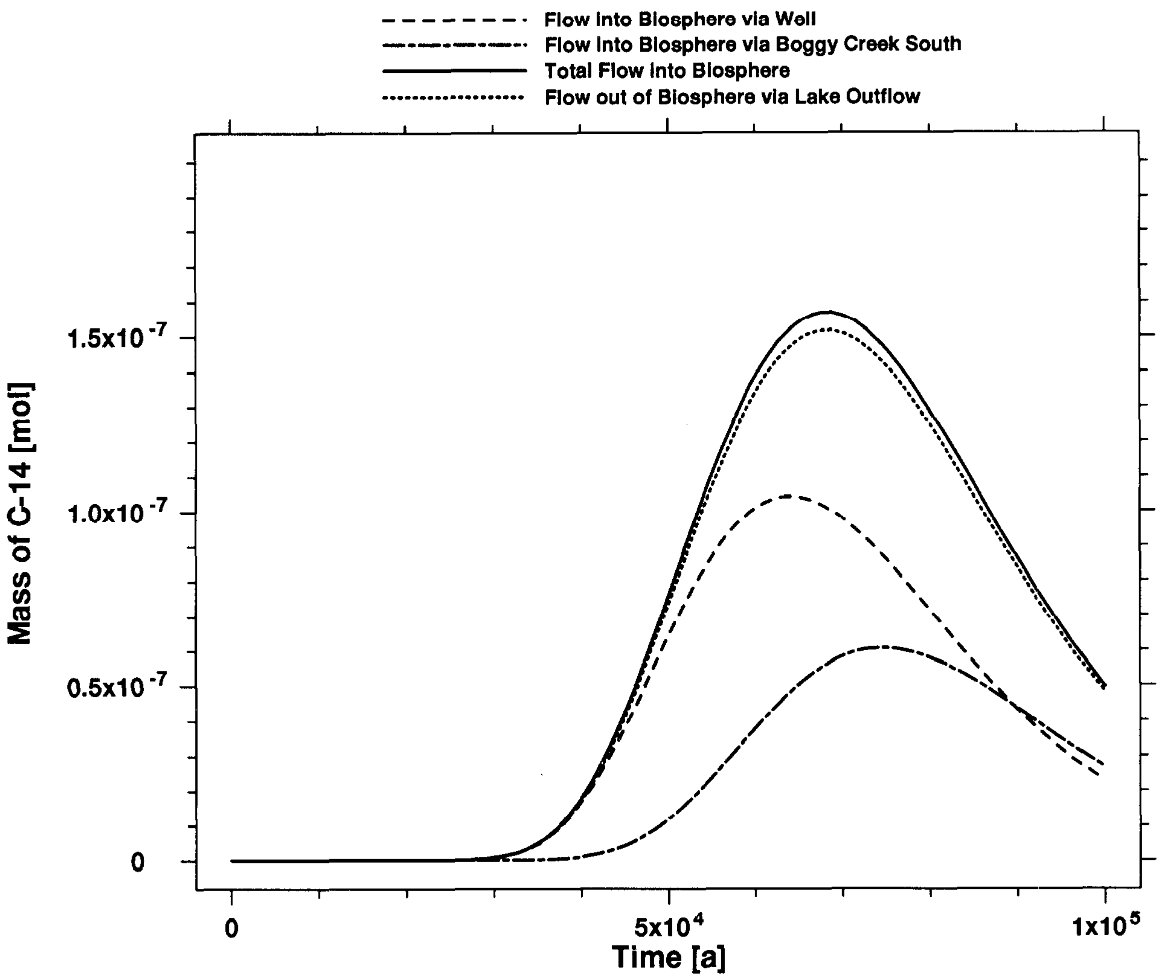

FIGURE D-35: Flows of ^{14}C in and out of the Modelled Biosphere

These curves show the ^{14}C flow in the modelled part of the biosphere for the median-value simulation. The topmost curve shows the total flow in; it is the sum of the bottom two curves, which represent flows in from Boggy Creek South and the well. The curve second from the top shows the total flow of ^{14}C out of the modelled portion of the biosphere, resulting from outflow in lake water.

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important to the operation of the system model and that are often obscured in a set of randomly sampled simulations.

Other sensitivity analyses on the individual models are described in the primary references on the vault model (Johnson et al. 1994), the geosphere model (Davison et al. 1994) and the biosphere model (Davis et al. 1993). We have compared corresponding results from these analyses with our sensitivity analyses for the median-value simulation (Sections 6.3.3 in the main text and D.6 to D.8 in Appendix D) to ensure that there is concurrence in the lists of important parameters and in our understanding of why they are important.

Some differences can be observed, and all can be attributed to the different scopes of the studies: the primary references on the vault model (Johnson et al. 1994), the geosphere model (Davison et al. 1994) and the biosphere model (Davis et al. 1993) focus on the individual models, whereas our study deals with the integrated system model. For example, we identify the size of the critical group as an important parameter for the system model (Section 6.3.3 in the main text), but it is not an important parameter in the biosphere model alone. This apparent disparity arises because the importance of the parameter to the system model derives from its effect on contaminant movement in the geosphere and to the well (Sections D.7.2 and D.7.5). It is not an important parameter in the biosphere-only study (Davis et al. 1993) because that study does not include variations in flows of contaminants through the geosphere.

D.5.2 OBJECTIVE FUNCTIONS USED IN THE ANALYSIS

As used here, an objective function is one of the variables calculated by SYVAC3-CC3 that describes an important endpoint. One important group of endpoints is the ADEs.

Section 6.3 in the main text shows that, in the median-value simulation, doses from ^{14}C and ^{129}I dominate the maximum ADEs up to 10^5 a. Thus we concentrate the detailed sensitivity analysis of the system model on three objective functions: the total ADE, and the ADE resulting from ^{14}C and the ADE resulting from ^{129}I. Most of the analysis is also concentrated on 10^5 a rather than 10^4 a, because

- There are more nonzero impacts on the critical group up to 10^5 a than up to 10^4 a in our system model because more contaminants reach the biosphere over the longer time period. Thus the statistics for the 10^5-year model responses are more reliable, because they are based on more nonzero data points.

- It is conservative to choose the longer period, in the sense that the maximum ADEs observed for times up to 10^5 a are larger in our system model than the maximum ADEs up to 10^4 a. Because we use maxima over time, the maxima up to 10^5 a are upper bounds on the maxima up to 10^4 a.

- Analyses using a longer time period tend to identify parameters that are important in attenuating ADEs, rather than important in merely delaying the arrival of contaminants in the biosphere.

We also examine several other objective functions in association with the vault, geosphere and biosphere models. They are

- Performance measures for the vault. For ^{129}I, the vault performance measure is defined as the total estimated amount of ^{129}I released from the vault up to 10^5 a. A similar measure is defined for ^{14}C.

- Performance measures for the geosphere. For ^{129}I, the geosphere performance measure is defined as the total amount of ^{129}I that leaves the geosphere divided by the total amount of ^{129}I that enters the geosphere, over 10^5 a. A similar performance measure is defined for ^{14}C.

- Performance measures for the biosphere. For ^{129}I, the biosphere performance measure is defined as the integral, up to 10^5 a, of the ADE from ^{129}I divided by the total amount of ^{129}I that enters the biosphere for times up to 10^5 a. A similar performance measure is defined for ^{14}C.

These ancillary objective functions serve to isolate particular components of the system model, and thus provide additional information on important parameters and features.

A number of other objective functions were considered, such as concentrations of radionuclides and chemically toxic contaminants in water, soil and air, and the estimates of dose to nonhuman biota. They were not examined in detail because we believe the ADEs and performance measures provide a satisfactory basis for understanding the median-value simulation.

Section 6.3.3 identifies the parameters that are important because of their effects on ADEs. Sections D.6 to D.8 (Appendix D) list some additional parameters that are important because of their effects on the performance measures for the vault, geosphere and biosphere models.

D.5.3 DETAILS OF THE METHOD

The first step in sensitivity analysis is to screen the several thousand parameters to select for further study only those that, when changed, cause a significant change in the chosen objective functions. The major tool used is iterated fractional factorial analysis, described in Section A.4 in Appendix A. This method can typically screen several thousand parameters, using only a few hundred simulations, in situations where a few parameters dominate the rest (Andres and Hajas 1993). Our experience demonstrates that this method is a reliable screening tool when supported with expert judgment.

The iterated fractional factorial method employs sets of simulations in which model parameters are given selected values, designed to determine the effects of the changes on the chosen model output using a practical number of simulations. In Section 6.3.3.1 in the main text, we noted that three general classes of input parameters are examined:

- sampled parameters that may have any value from a continuous range of feasible values (when sampled during the probabilistic analysis);

- switch parameters that have a value from one of several possible values (and that are used to select one option from a group of mutually exclusive options in a simulation for the probabilistic analysis); and

- constant parameters that normally take on a single fixed value.

We make the distinction because it influences how sensitivity analysis is performed and how the results are interpreted (as discussed below). From computer simulation and mathematical viewpoints, switches and constant parameters need not be distinguished from one another, nor from any other variable parameter. All are types of parameters that are used by the model of the system and that are input to SYVAC3-CC3 to perform simulations. All are described using PDFs in the probabilistic analysis. Sampled parameters are described using one of many possible PDFs, such as normal, uniform and lognormal PDFs (Figure A-6 in Appendix A). Switches generally use piecewise uniform PDFs, such that each separate range of the distribution defines the probability of one option. Finally, constant parameters use a constant PDF, which defines the single fixed value of the parameter.

In selecting values for the model parameters, we employed the following consistent approach:

- For all sampled parameters, small-variation studies use parameter values that are fixed in different simulations at the 0.475 or 0.525 quantiles of their PDFs. (There is a one-to-one mapping of a parameter value with its quantile. The smallest and largest possible values of the parameter correspond to the 0 and 1 quantiles. In 1000 random samples of a parameter from its PDF, about 475 values would be less than or equal to the value that corresponds to the 0.475 quantile. Similarly, 525 values on average would be less than or equal to the value corresponding to the 0.525 quantile.)

  With this choice, the effects of a variable parameter on the chosen objective function are examined for values that are near its median value and that deviate above and below the median value by amounts that are equally likely to occur (based upon its PDF). This method of defining the changes to the parameters permits direct comparison of the effects of parameters that have different physical units and different probability distributions. Studies using the 0.475 and 0.525 quantiles are for a two-level design (Section A.4 in Appendix A). Other screening studies involve a three-level design, using the 0.425, 0.500 and 0.575 quantiles.

- For all sampled parameters, full-range studies examine a broader range of possible values for each parameter. These studies examine variations using the 0.0, 0.01, 0.99 and 1.0 quantiles to screen for parameters whose effects are important when they are given values spanning their full range of uncertainty. The full-range studies also involve two- and thee-level designs.

- For all switch parameters, values are chosen that encompass all acceptable options associated with the switch. For example, there are two possible values for the switch that selects the source of domestic water used by the critical group: one value corresponds to the use of well water and the other to the use of lake water. Similarly, the switch that selects the type of garden soil has four possible values to cover four options (for sand, clay, loam and organic soils). Sensitivity analysis of the median-value simulation includes examination of all possible values of each switch parameter or all options allowed by the switches.

- For a constant parameter, sensitivity analysis uses feasible values selected from near its fixed value. Where possible, the selected values are 10% above and below the fixed value. For some parameters, 10% variations are not feasible because they would result in an inconsistent model. This occurs for parameters such as those defining the coordinates of the nodes for the network of segments in the geosphere: a 10% variation would lead to significant incompatibilities in the description of the groundwater flow field and, therefore, we use smaller variations.

Once the important parameters have been identified, the next step in our sensitivity analysis is to demonstrate how these important parameters affect the estimated responses of the system model. These effects are inferred from another series of simulations involving systematic variation of the important parameters. Typically, for an important sampled parameter

- To study effects near the median values, the parameter is given a series of values that range between its 0.475 and 0.525 quantiles, whereas all other parameters are fixed at their median values. To study effects over the full range of values, the parameter is given values corresponding to its 0.0, 0.02, 0.05, 0.10, 0.20, 0.30, 0.40, 0.51, 0.60, 0.70, 0.80, 0.90, 0.95, 0.98 and 1.0 quantiles, whereas all other parameters are fixed at their median values. (The 0.0 and 1.0 quantiles are excluded for parameters whose distributions are not bounded or are very broad. In addition, other intermediate quantiles are used if needed to better define a curve of effect versus parameter value.) A set of simulations is then performed using each specified quantile, and plots of the ADEs versus parameter values show explicitly the effects of the parameter.

For important switch parameters, we typically generate simulations for each possible value of the switch. For constant parameters, we generate simulations where the "possible" values of the constant are its fixed value and selected values above and below its fixed value.

Sections D.6 to D.8 of Appendix D discuss these effects for the vault, geosphere and biosphere models.

D.6 SENSITIVITY ANALYSIS OF THE VAULT MODEL

D.6.1 IMPORTANT PARAMETERS OF THE VAULT MODEL

The screening of parameters of the system model identifies six important parameters used in the vault model (Table 6-2 in the main text). They are important in the median-value simulation in the sense that small variations near their median values result in significant changes to the maximum ADEs from ^{14}C and ^{129}I up to 10^5 a. The six important parameters are

- the buffer anion correlation parameter (which correlates the values of the buffer diffusion coefficient and the buffer capacity factor for anionic species (Johnson et al. 1994));

- the initial inventory of ^{129}I in used fuel;
- the initial inventory of ^{14}C in used fuel;
- the instant-release fraction from used fuel for ^{14}C;
- the groundwater velocity scaling factor (a dimensionless, multiplicative factor used to describe the uncertainty in groundwater velocities in the geosphere (Davison et al. 1994)); and
- the tortuosity of the lower rock zone (a measure of the increased distance for diffusive transport caused by the winding nature of the interconnected aqueous pathway).

The last two parameters are normally associated with the geosphere model, but they also affect the vault model through the linkages between the vault and geosphere models (Section 5.3 in the main text).

For variation of all sampled parameters over their entire range of possible values, seven parameters used in the vault are important (Table 6-3 in the main text); the six listed above and

- the instant-release fraction from used fuel for ^{129}I.

Finally, another fractional factorial screening study was directed at the vault performance measures. The vault performance measure for ^{129}I is defined to be the total estimated amount of ^{129}I released from the vault up to 10^5 a. It represents the effectiveness of the vault as a barrier to the movement of ^{129}I, with smaller values corresponding to greater effectiveness. A similar performance measure is defined for ^{14}C. This study also identified as important the seven parameters listed above.

Table D-12 shows the ratios of the largest to the smallest vault performance measures for ^{129}I and for ^{14}C when we vary one important parameter at a time over its range of possible values (based on its PDF). The relative effects of each parameter can be shown by comparing the ratios in the table; for example,

- The initial inventories of ^{14}C and ^{129}I have the largest effect on changing the total amounts of these nuclides released from the vault over 10^5 a. The differential effects between the two nuclides can be attributed to the different ranges of initial inventories that are examined (^{14}C has the largest range of possible values).
- The instant-release fractions from used fuel for ^{129}I and ^{14}C also have large effects. As before, the differential effects between the two nuclides are attributed to their different ranges of possible values.

TABLE D-12

RELATIVE IMPORTANCE OF VAULT PARAMETERS ON ESTIMATED RELEASES FROM THE VAULT*

Parameter	Release Ratio for: ^{129}I	^{14}C
Initial inventory of ^{129}I in used fuel	32	1
Instant-release fraction from used fuel for ^{129}I	18	1
Buffer anion correlation parameter	18	43
Groundwater velocity scaling factor	11	15
Tortuosity of the lower rock zone	3	3
Initial inventory of ^{14}C in used fuel	1	100
Instant-release fraction from used fuel for ^{14}C	1	25

* The parameters listed are those that have the most significant effects on the total estimated releases of ^{14}C and ^{129}I from the vault for times up to 10^5 a. The release ratios are, for each nuclide, the ratios of the largest to the smallest releases that are calculated when each parameter is separately varied over its range of possible values and when all other parameters are fixed at their median values. (The values actually used correspond to the following quantiles: 0.0, 0.02, 0.05, 0.1, 0.2, 0.3, 0.4, 0.51, 0.6, 0.7, 0.8, 0.9, 0.95, 0.98 and 1.0.) A release ratio of unity implies no effect.

- Other important parameters, such as the buffer anion correlation parameter, groundwater velocity scaling factor and tortuosity of the lower rock zone, are not nuclide-specific. They each affect releases of ^{14}C and ^{129}I in the same way; for instance, increasing the buffer anion correlation parameter increases the estimated releases of both nuclides. The results again show a different degree in magnitude for the two nuclides that can be attributed to the relative differences in half-lives for ^{14}C and ^{129}I.

- Parameters that describe characteristics of one nuclide have no effect on ratios of other nuclides. Thus the ratio for ^{14}C is unity (that is, there is no difference) when the initial inventory of ^{129}I is changed.

Finally, the relative importance of the parameters depends on whether the response examined is total estimated releases from the vault or the maximum ADEs. A comparison of the results in Tables D-12 and 6-3 (in the main text) shows that full-range variations of two parameters have a much greater effect on the maximum ADE than on total estimated releases from the vault: the groundwater velocity scaling factor and the tortuosity of the lower rock zone. The reasons for these effects are described in Section D.6.4.

D.6.2 EFFECTS OF INVENTORIES AND INSTANT-RELEASE FRACTIONS

Changes in the initial inventories of ^{14}C and ^{129}I cause the greatest changes to the total releases from the vault: for example, Table D-12 shows the total release of ^{14}C to 10^5 a increases by a factor of 100 when its initial inventory in used fuel is increased from its minimum value to its maximum value.

This sensitivity arises because the total release of a contaminant from the vault is proportional to its inventory, provided that the contaminant does not exceed its solubility limit and precipitate in the vault buffer. Solubility limits for ^{14}C and ^{129}I are extremely large and do not affect their releases in the median-value simulation. (In contrast, solubility limits for ^{99}Tc can be relatively small, and releases of ^{99}Tc are bounded in the median-value simulation and in many other simulations.) Figures D-36 and D-37 show how the total releases of ^{14}C and ^{129}I from the vault vary with changes in their initial inventories (all other parameters are fixed at their median value). As noted in Section 6.3.3.2 in the main text, ^{14}C shows a greater effect than ^{129}I in Table D-12 because its initial inventory in used fuel has a greater range of possible values.

The instant-release fraction from used fuel determines the amount of the initial inventory of a contaminant that is released within the container at the instant of container failure. Because the releases from the vault of ^{14}C and ^{129}I are dominated by their instantly released inventories (over the entire time period covered by the simulations), the instant-release fractions for ^{14}C and ^{129}I have an effect similar to their initial inventories. This effect is illustrated in Figures D-38 and D-39, which show the total releases of ^{14}C and ^{129}I from the vault as a function of their instant-release fractions from used fuel. Carbon-14 shows a greater effect than ^{129}I in Table D-12 because it covers a greater range of values.

Curves similar to those in Figures D-36 to D-39 are obtained when the maximum ADEs resulting from ^{129}I and ^{14}C are plotted against initial inventories and instant-release fractions from used fuel. These parameters act as scaling factors in the median-value simulation; that is, they change the magnitude of estimated model responses by the same value at all times. Thus increases in these parameters result in proportional increases in total releases from the vault and the maximum ADEs for ^{129}I and ^{14}C. The increases may not be identically proportional if processes such as precipitation and isotopic dilution are important.

D.6.3 EFFECTS OF THE BUFFER ANION CORRELATION PARAMETER

The buffer anion correlation parameter is used to correlate the values of the buffer diffusion coefficient and the buffer capacity factor for all contaminants in the vault that are expected to form anionic species in groundwater (Johnson et al. 1994). Both ^{14}C and ^{129}I are modelled as anionic species.

A single buffer anion correlation coefficient is required to determine the diffusion coefficients and capacity factors of all anionic contaminants.

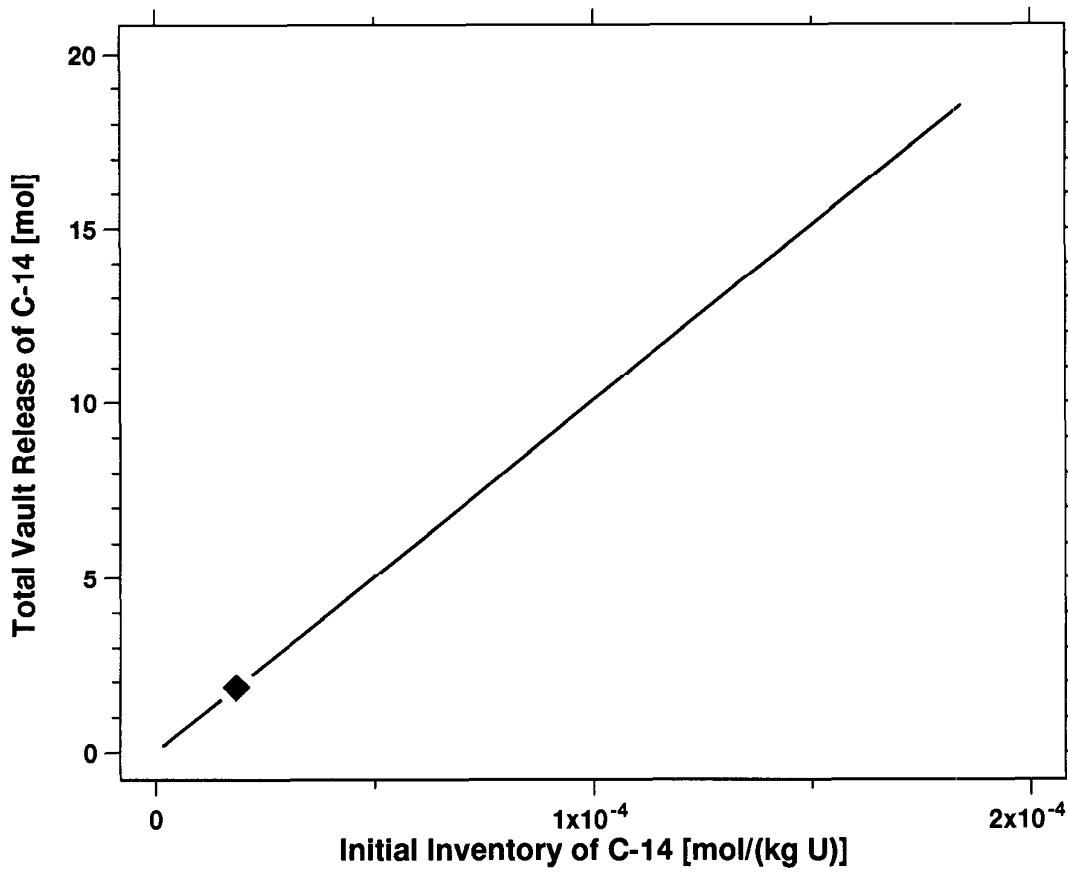

FIGURE D-36: Effect of ^{14}C Inventory on Releases from the Vault

The curve shows the total release of ^{14}C from the vault up to 10^5 a, as a function of its initial inventory in used fuel and when all other parameters are fixed at their median value. The initial inventory of ^{14}C in used fuel is varied throughout the range defined by its PDF; the symbol on the curve locates its median value.

The correlation is positive, meaning that both the diffusion coefficient and capacity factors tend to increase or decrease in unison. This dependence is based on the experimental observations that as the porosity of the buffer decreases, the storage capacity and the diffusion capability for anions in the buffer decrease together. (The primary reference for the vault model (Johnson et al. 1994) describes these observations.)

Figure D-40 shows the effect of the buffer anion correlation parameter on total estimated release of ^{129}I from the vault, where the correlation parameter varies over its entire range (9.0×10^{-7} to 3.6×10^{-4}) and all other parameters are fixed at their median values. (Similar results are observed for ^{14}C except for small differences attributable to its smaller half-life). The curve shows an overall variation in total release of more than a factor of 10, and a maximum release near a parameter value equal to 1×10^{-4}.

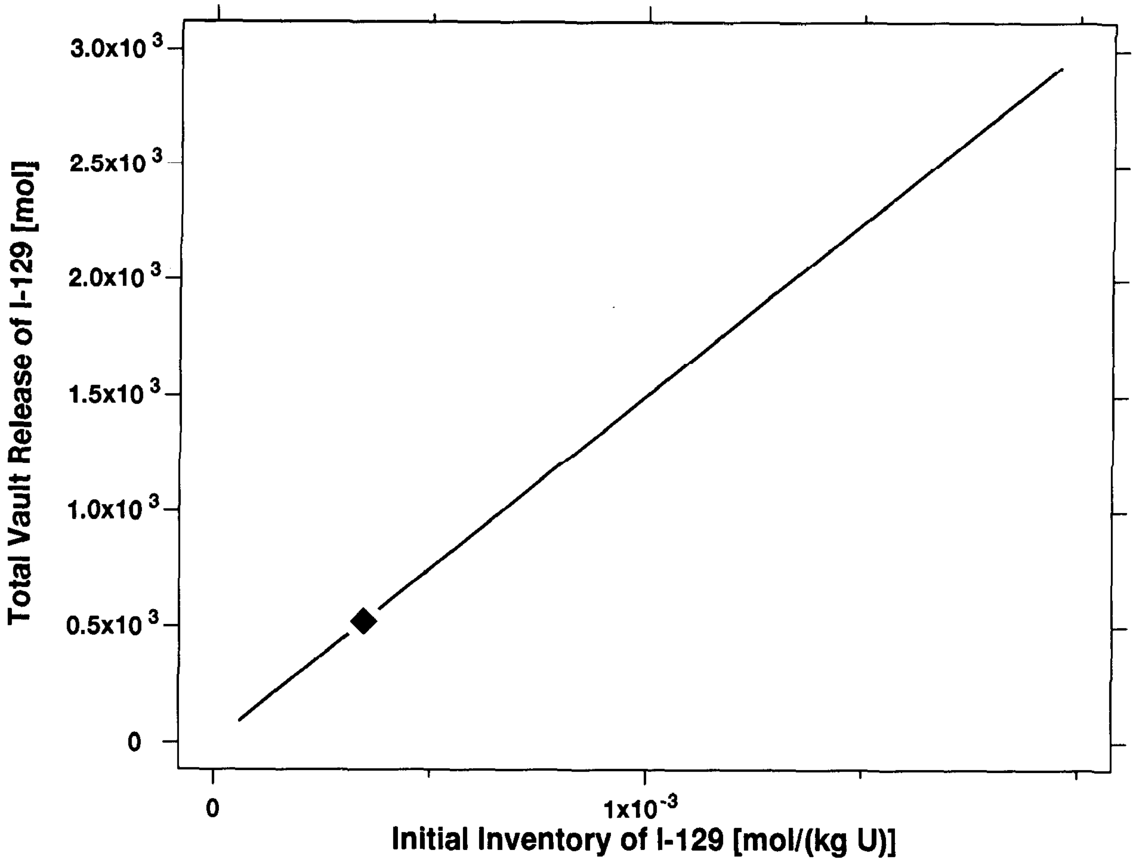

FIGURE D-37: Effect of ^{129}I Inventory on Releases from the Vault

Comments are as for the previous figure, except that the data are for ^{129}I.

The shape of the curve arises because changing the buffer anion correlation parameter has two counteracting effects on contaminant releases from the buffer (which is reflected in the releases from the vault). For an anionic contaminant, an increased buffer anion correlation parameter corresponds to a higher diffusion coefficient and a larger capacity factor, and

- Increased rates at which the contaminant is drawn into the buffer from the containers; and

- Decreased rates of contaminant release from the buffer because of delays in transport through the buffer (more accurately, this second effect delays contaminant transport, and thereby reduces early releases).

The first effect is approximately proportional to the magnitude of both parameters, whereas the second effect is proportional to the ratio of the diffusion coefficient to the capacity factor: as this ratio decreases, the delay time increases.

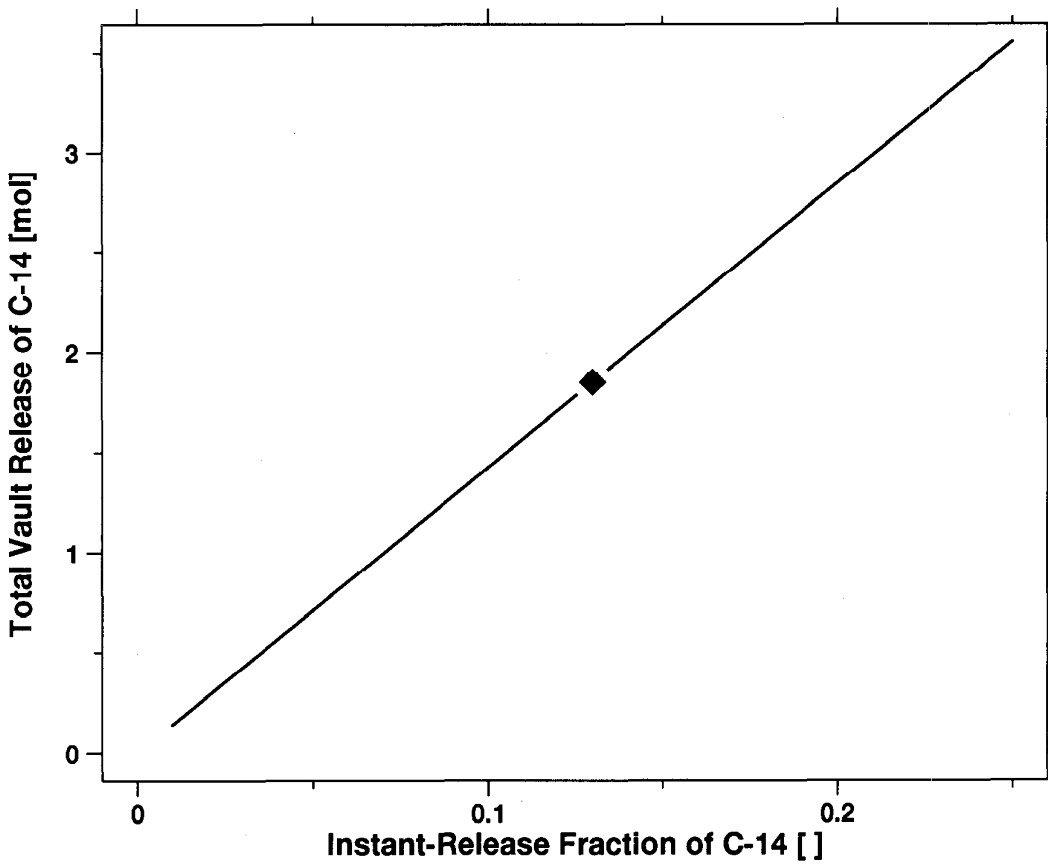

FIGURE D-38: Effect of ^{14}C Instant-Release Fraction on Releases from the Vault

The curve shows the total release of ^{14}C from the vault up to 10^5 a, as a function of its instant release fraction from used fuel and when all other parameters are fixed at their median value. The instant-release fraction of ^{14}C is varied throughout the range defined by its PDF; the symbol on the curve locates its median value.

Either of the above two effects may dominate the other. In fact, both extremes are observed in these studies of the median-value simulation because of the range of possible values of the buffer anion correlation parameter. For increased values of the parameter near its smallest values, the first effect dominates; that is, releases from the buffer (and the vault) increase as the correlation parameter increases. This trend does not continue indefinitely. As noted above, increasing the buffer anion correlation parameter leads to increases in both the capacity factor and diffusion coefficient. However, the range of variation of the diffusion coefficient is less than that of the capacity factor. Therefore, the <u>ratio</u> of the diffusion coefficient to the capacity factor decreases as these two parameters are increased from their lowest to greatest values over their respective ranges. Thus the second effect tends to become more important for large values of the buffer anion correlation parameter.

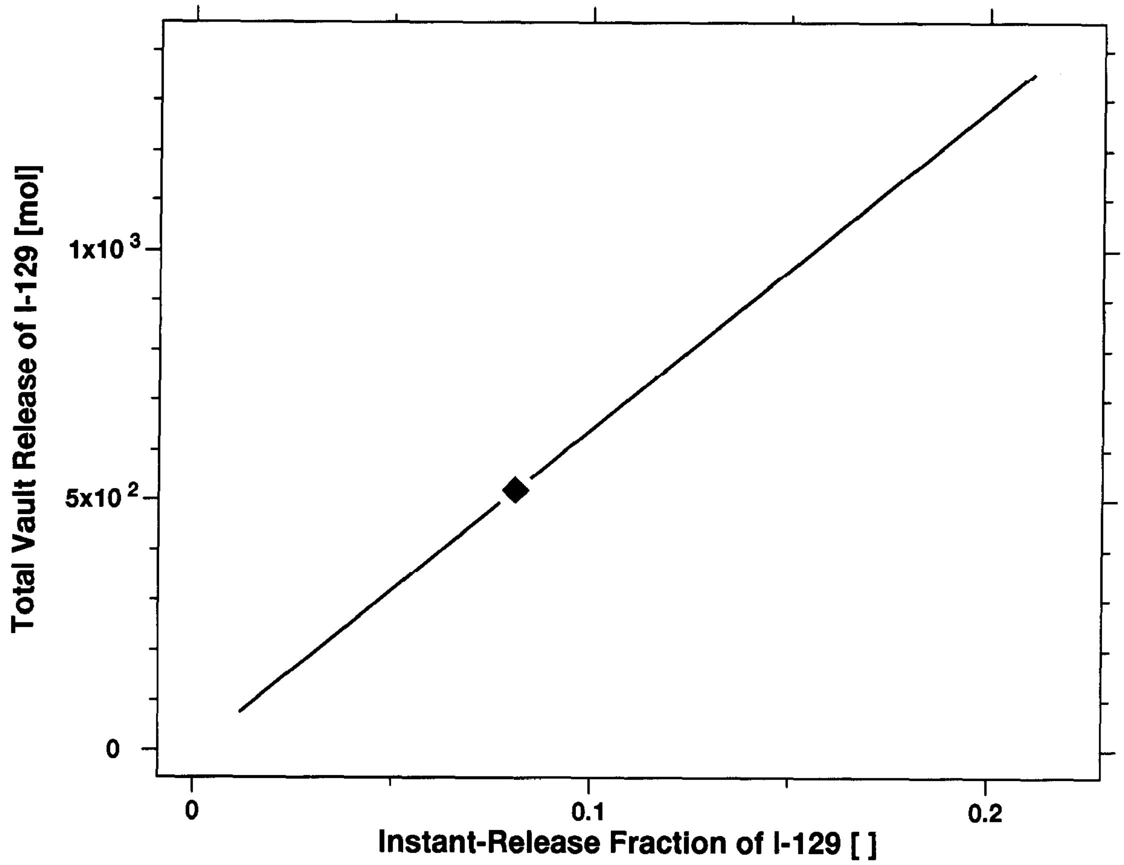

FIGURE D-39: Effect of ^{129}I Instant-Release Fraction on Releases from the Vault

Comments are as for the previous figure, except that the data are for ^{129}I.

For the median-value simulation, the range of values for the capacity factor and diffusion coefficients for ^{14}C and ^{129}I are such that both effects are observed. Hence as these parameters increase, the control over the amount released shifts from the rapid movement of contaminant into the buffer to the increased delay time in the buffer. Thus the curve in Figure D-40 shows a maximum value in total estimated release.

A similar effect is possible for the backfill. However, it is not observed because of the different ranges of possible values of the transport parameters for the buffer and the backfill. In the backfill, the capacity factor and diffusion coefficient for ^{129}I both vary by only a factor of 1.5, whereas in the buffer they vary by factors of 4000 and 400.

Plots of the maximum ADE versus the buffer anion correlation parameter have a curve similar to that in Figure D-40.

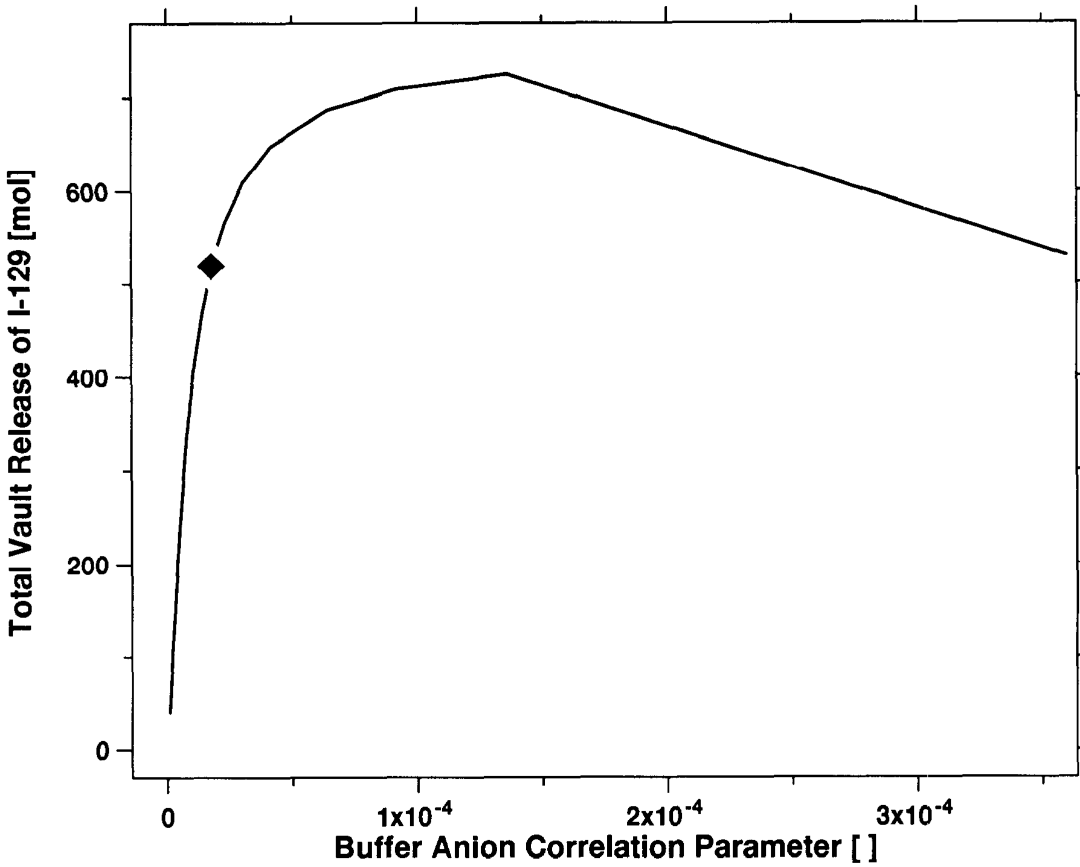

FIGURE D-40: Effect of the Buffer Anion Correlation Parameter on ^{129}I Releases from the Vault

The curve shows the total release of ^{129}I from the vault up to 10^5 a, as a function of the buffer anion correlation parameter (a dimensionless correlation parameter) and when all other parameters are fixed at their median value. The buffer anion correlation parameter is varied throughout the range defined by its PDF; the symbol on the curve locates its median value.

D.6.4 EFFECTS OF THE PROPERTIES OF THE SURROUNDING ROCK

The groundwater velocity scaling factor and the tortuosity of the lower rock zone are parameters normally associated with the geosphere model; however, they are also used in the calculation of the mass transfer coefficient at the vault-geosphere boundary (Section 5.3 in the main text). The mass transfer coefficient is a measure of the relative conductance to contaminant transport of the rock adjacent to the vault.

Figures D-41 and D-42 illustrate the effects of the groundwater velocity scaling factor and the tortuosity of the lower rock zone on estimated releases of ^{129}I from the vault for times up to 10^5 a. (Similar results are observed for ^{14}C.)

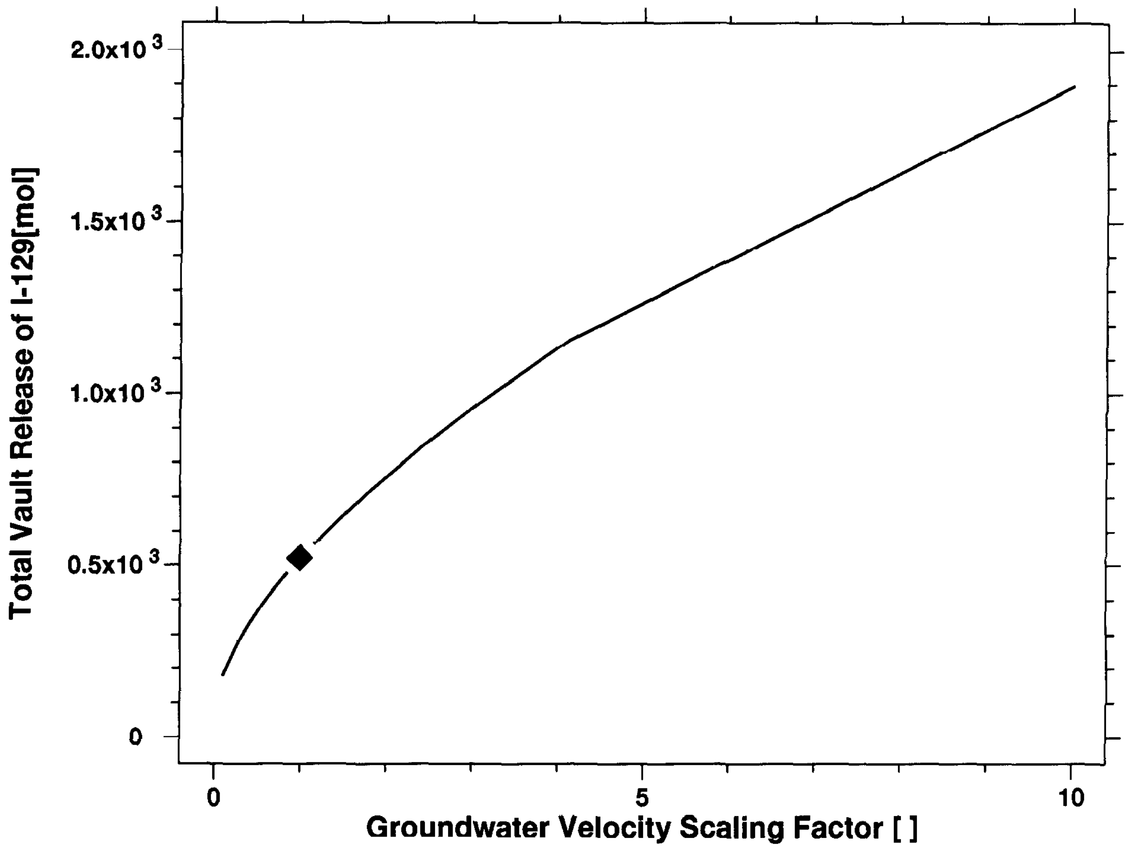

FIGURE D-41: Effect of the Groundwater Velocity Scaling Factor on ^{129}I Releases from the Vault

The curve shows the total release of ^{129}I from the vault up to 10^5 a as a function of the groundwater velocity scaling factor (a dimensionless parameter) and when all other parameters are fixed at their median value. The groundwater velocity scaling factor is varied throughout the range defined by its PDF; the symbol on the curve locates its median value.

Increasing the groundwater scaling factor increases the groundwater velocities in the rock surrounding the vault, which in turn tends to increase the mass transfer coefficient of the vault backfill, and thus to increase the total estimated release of ^{129}I. Increasing the tortuosity of the lower rock zone increases contaminant transport times in the rock surrounding the vault, which decreases the mass transfer coefficient, and thus causes a decrease in the total estimated release of ^{129}I.

These two parameters show complex effects on the ADE because they change the time dependence of estimated releases. Hence a change in the estimated total release from the vault to 10^5 a does not produce a proportional change in the estimate of the maximum ADE up to that time.

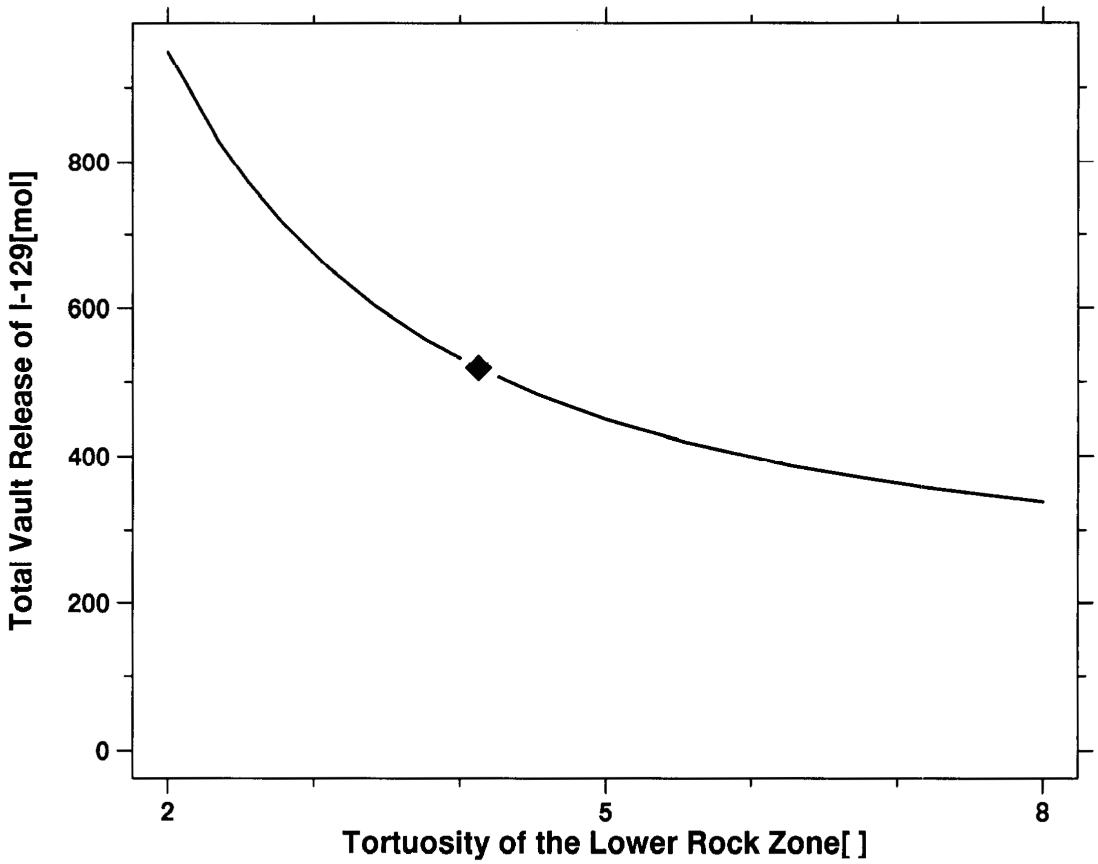

FIGURE D-42: Effect of the Tortuosity of the Lower Rock Zone on ^{129}I Releases from the Vault

The curve shows the total release of ^{129}I from the vault up to 10^5 a as a function of the tortuosity of the lower rock zone (a dimensionless parameter) and when all other parameters are fixed at their median value. The tortuosity of the lower rock zone is varied throughout the range defined by its PDF; the symbol on the curve locates its median value.

Moreover, these two parameters have strong effects in the geosphere (discussed in the following section), where they act to cause further delays in contaminant transport. Thus the importance of these two parameters is greater for the maximum ADEs (Table 6-3 in the main text) than for total estimated releases from the vault (Table D-12).

D.7 SENSITIVITY ANALYSIS OF THE GEOSPHERE MODEL

D.7.1 IMPORTANT PARAMETERS OF THE GEOSPHERE MODEL

The screening of parameters and features of the system model identified four important parameters used in the geosphere model (Table 6-2 in the main text). They are

- the tortuosity of the lower rock zone);

- the free-water diffusion coefficient for iodine;

- the groundwater velocity scaling factor (a dimensionless, multiplicative factor used to describe the uncertainty in groundwater velocities in the geosphere (Davison et al. 1994)); and

- the free-water diffusion coefficient for carbon.

These parameters are important in the median-value simulation in the sense that small variations near their median values result in significant changes to the maximum (up to 10^5 a) ADEs from ^{14}C and ^{129}I.

Section 6.3.3.5 in the main text notes that the ADEs are also sensitive to the closest distance between a vault room and fracture zone LD1. This is the waste exclusion distance, with a value of about 50 m. Because the orientation of the vault is fixed, the waste exclusion distance is a constant. Thus we cannot examine its effects in the same systematic fashion as we have done for other parameters. The development of derived constraints described in Sections 6.2 and 6.6 in the main text includes an analysis of the effects of different waste exclusion distances that obtain when the vault orientation is modified. Note, however, that the importance of the waste exclusion distance is implicitly included in the above list: the tortuosity of the lower rock zone and the groundwater velocity scaling factor both refer to properties of the rock and water within the waste exclusion distance.

For variation of all sampled parameters over their entire range of possible values, six parameters are identified as the most important (Table 6-3 in the main text). They are the four listed above, and

- the depth of the well and

- the number of persons per household (of the critical group).

This last parameter is normally associated with the biosphere model. However, it also affects the geosphere model because groundwater flows in the geosphere depend on the volume of water withdrawn from the well by the critical group.

Finally, another fractional factorial screening study was directed at the geosphere model alone, to examine the effects of system parameters on a measure of the performance of the geosphere. The geosphere performance measure for ^{129}I is defined as the ratio of the total amount of ^{129}I

released from the geosphere in 10^5 a to the total amount of ^{129}I released from the vault in 10^5 a. It represents the effectiveness of the geosphere as a barrier to the movement of ^{129}I: a smaller value corresponds to a more effective barrier. A similar performance measure is defined for ^{14}C.

This auxiliary screening identified as important the above six parameters and

- the thickness of the overburden.

Five additional parameters are somewhat important for ^{14}C but not for ^{129}I. They are the four switches selecting the source of the domestic water, the soil type, whether the garden is irrigated and the use of lake sediment as soil, and one parameter describing the thickness of the lake sediment. These four switches are generally associated with the biosphere model, and their effects are discussed in Section D.8. The effect of the thickness of the lake sediment is similar to that of the thickness of the overburden and is not discussed further here.

Table D-13 summarizes the dependence of the performance measure of the geosphere model on the seven important parameters listed above. The relative effects of each parameter can be shown by comparing the ratios in the table; for example,

- The relative importance of the parameters depends on whether the response examined is the maximum ADE (Tables 6-2 and 6-3 in the main text) or the geosphere performance measures (Table D-13).

- The tortuosity of the lower rock zone clearly has the largest effect on the geosphere performance measure for ^{129}I. Increasing the value of this parameter increases the effectiveness of the geosphere as a barrier to ^{129}I movement.

- The tortuosity of the lower rock zone also has a large effect on the geosphere performance measure for ^{14}C. As for ^{129}I, increasing the value of this parameter increases the effectiveness of the geosphere as a barrier to ^{14}C movement.

- The groundwater velocity scaling factor is clearly the most important parameter affecting the geosphere performance measure for ^{14}C, but it has a much smaller effect for ^{129}I. In the discussion below, this difference in importance is related to the different half-lives of ^{14}C and ^{129}I.

In the following discussion, we first describe the characteristics of the well, because there is a complex interplay of parameters that control the effects of the well. We then discuss the effects of the important parameters on estimated releases from the geosphere model and on the ADEs.

TABLE D-13

RELATIVE IMPORTANCE OF PARAMETERS ON GEOSPHERE PERFORMANCE MEASURES*

Parameter	Ratios of Geosphere Performance Measure for: ^{129}I	^{14}C
Tortuosity of the lower rock zone	1200.	47000.
Free-water diffusion coefficient for iodine	39.	1.0
Groundwater velocity scaling factor	7.3	130000.
Thickness of the overburden	1.3	2.1
Number of persons per household	1.1	4.0
Free-water diffusion coefficient for carbon	1.0	240.
Depth of the well	1.0	1.8

* The parameters listed are those that have the greatest effect on measures of the performance of the geosphere as a barrier to the transport of ^{129}I and ^{14}C. The two columns on the right-hand side show ratios of the largest to the smallest performance measures for ^{14}C and ^{129}I that are calculated when each parameter is varied separately over its range of possible values and when all other parameters are fixed at their median values. (For most parameters, the values actually used correspond to the following quantiles: 0.0, 0.02, 0.05, 0.1, 0.2, 0.3, 0.4, 0.51, 0.6, 0.7, 0.8, 0.9, 0.95, 0.98 and 1.0. For "Number of persons per household" (of the critical group), values used ranged from 1 to 36.) A ratio of unity indicates the parameter has no effect.

D.7.2 EFFECTS OF CHARACTERISTICS OF THE WELL

The geosphere model includes a well that is located near the site of the reference disposal vault. In the median-value simulation (and in about 50% of the randomly sampled simulations), it supplies the domestic water used by the critical group. It may also supply water used to irrigate the garden.

The well can be classified in several broad schemes. One is whether the well is an overburden or bedrock well:

- Overburden wells do not extend past the overburden that overlies the rock of the geosphere. We assume that only surface water reaches the well and that the concentrations of contaminants in this surface water are identical to concentrations in lake water.

- Bedrock wells extend past the overburden. We assume that they are sited above the centre line of the contaminant plume moving upwards along fracture zone LD1 and that they are located at a position along the centre line such that the bottom of the well intersects LD1 (Section 5.4 in the main text). In this case, the well will gather contaminated groundwater moving upwards along fracture zone LD1 that has collected contaminants released from the vault. It may also gather surface water infiltrating downwards along LD1.

Another classification is based on the use of well water. The characteristics of the well are such that it can usually supply enough water for domestic use by the critical group. It may also supply enough water for irrigation of the garden (use of the well for irrigation is determined by the switch that selects the irrigation option). If the demand for domestic and irrigation water is sufficiently large, then the physical capacity of the well to supply water may be exceeded. When the provisional demand on the well exceeds its capacity, we reduce the demand by first assuming that the critical group obtains its irrigation water from the lake. If the demand still exceeds capacity, we then assume that the critical group also obtains its domestic water from the lake. In the median-value simulation, the well capacity is sufficient to supply both domestic and irrigation water, although there are some simulations encountered in the sensitivity analysis where water demand exceeds well capacity.

The principal parameters controlling the characteristics of the well are the groundwater velocity scaling factor, the depth of the well, and the volume of water drawn from the well (which depends on the number of persons making up the household of the critical group). In the median-value simulation, the value of the groundwater velocity scaling factor is unity and the depth of the well is 37 m. It is a bedrock well because the overburden is only 7.4 m deep. Well water is used for domestic and irrigation use by three people who make up the household of the critical group. The well supplies 1330 m^3 water per year, of which 1290 and 40 m^3/a are from groundwater moving upwards and downwards along LD1.

Systematic changes to these parameters have the following effects:

- <u>Groundwater velocity scaling factor</u>. Increases in values for this parameter correspond to increased availability of water in LD1 and the surrounding rock to meet the well demand of 1330 m^3/a. Thus the well draws water from a smaller radius, thereby capturing a smaller portion of the contaminant plume moving up LD1. Figure D-43 shows the effect of the groundwater velocity scaling factor on the fraction of the contaminant plume, moving upwards in LD1, that is captured by the well (all other parameters are fixed at their median values). As the scaling factor is increased from about 0.24 to its maximum value of 10, the plume capture fraction gradually decreases from about 0.7 to 0.03. This gradual decrease reflects the smaller radius from which the well draws its water.

  When the scaling factor is below about 0.24, the effect of the well capacity influences the results. At the minimum value of the scaling factor (0.1), the well capacity would be exceeded, and thus the volume of water drawn from the well is reduced by drawing irrigation water from the lake. The reduced volume drawn from the well then reduces the plume capture fraction to about 0.65. Thus the curve shows a maximum when the groundwater velocity scaling factor is near a value of 0.24.

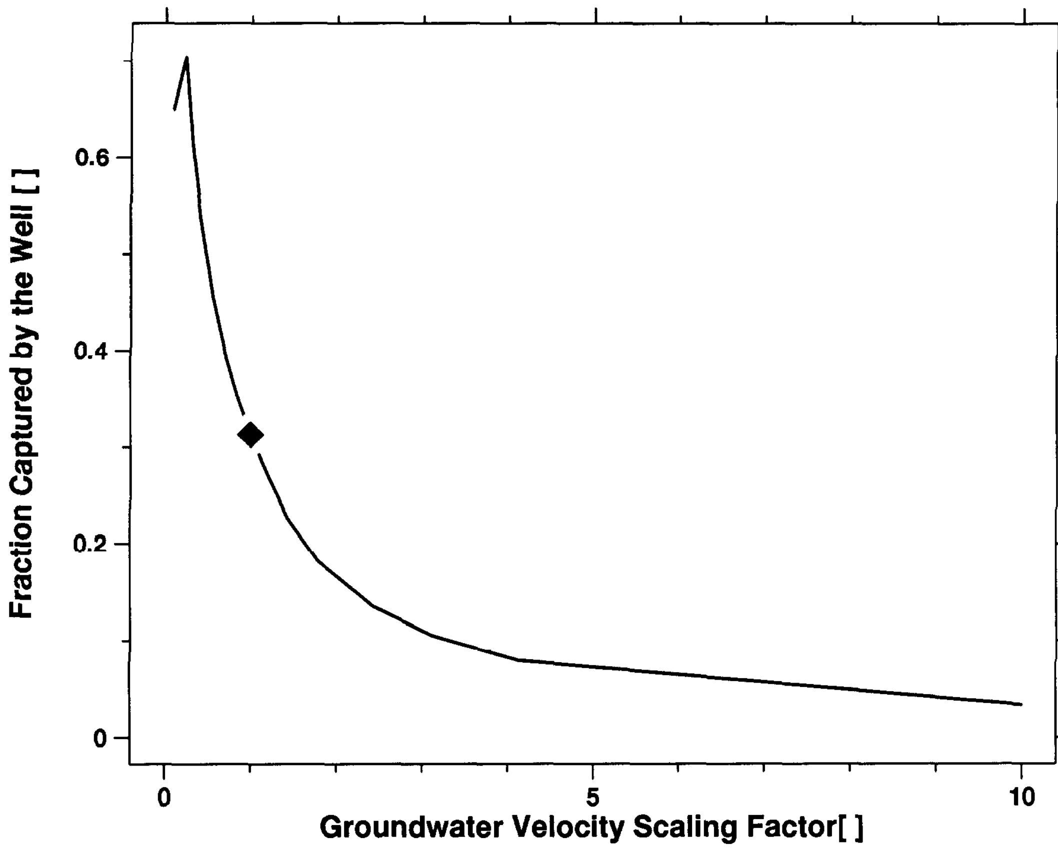

FIGURE D-43: Effect of the Groundwater Velocity Scaling Factor on Contaminant Capture by the Well

The curve shows the effect of the groundwater scaling factor (a dimensionless parameter) on the estimated fraction of contaminants captured by the well. In general, greater values of the scaling factor correspond to increased availability of groundwater for the well, thus the well draws water from a smaller radius and captures less of the contaminant plume. This pattern fails for small values of the groundwater velocity scaling factor (less than about 0.2), because of the effects of well capacity (see text). The groundwater velocity scaling factor is varied throughout its range of possible values, and all other parameters are fixed at their median values. The symbol in the curve locates its median value.

- Depth of the well. This parameter affects the proportions of deep groundwater and surface groundwater that enter the well. As noted above, overburden wells that extend only into the overburden (7.4 m deep in the median-value simulation) draw only surface water. Deeper wells intersect LD1 and draw both surface water and groundwater. Figure D-44 shows the volume of surface water drawn into the well as a function of the depth of the well, for depths greater than 7.4 m and with all other parameters fixed

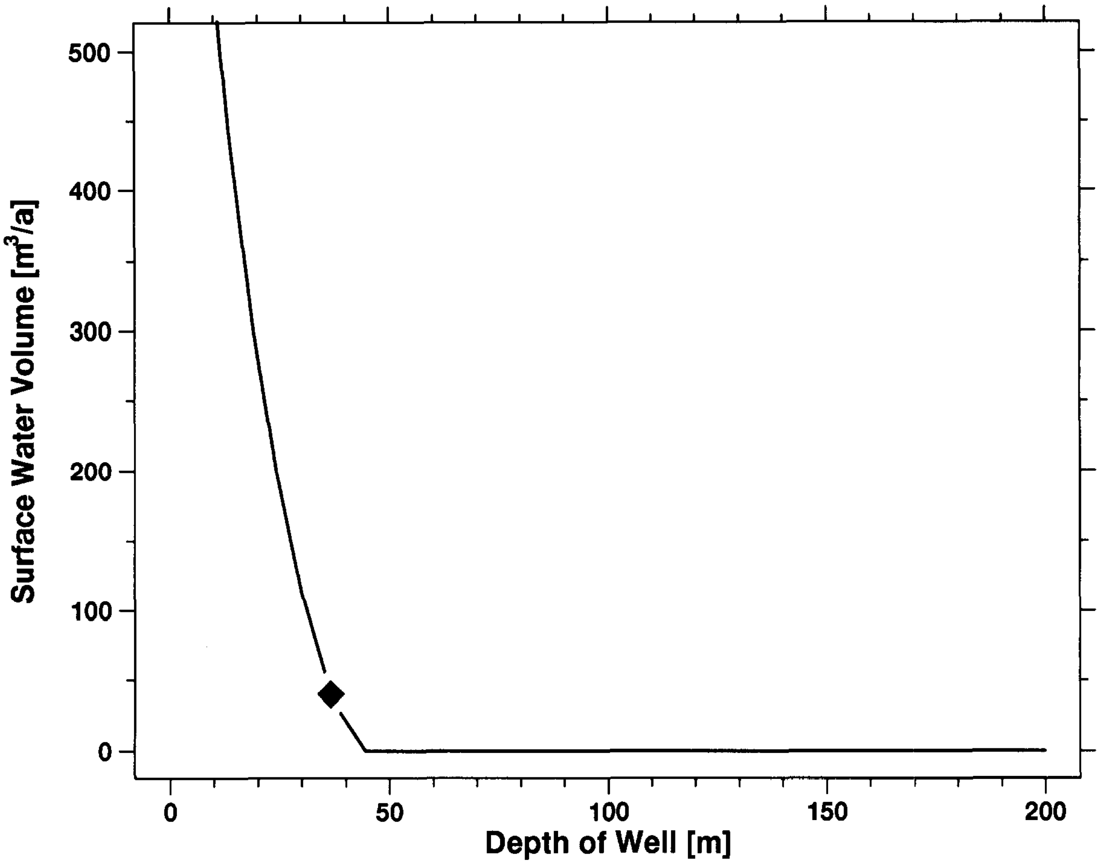

FIGURE D-44: Volume of Surface Water Drawn into Bedrock Wells Versus Depth of the Well

The curve shows the estimated volume of surface groundwater that is drawn into bedrock wells as a function of the depth of the well. Bedrock wells are those that extend beyond the overburden to intersect fracture zone LD1; thus the curve starts at a well depth of 7.4 m (the thickness of the overburden in the median-value simulation). The well supplies a total of 1300 m^3 of water per year, with the water originating from deep groundwaters travelling up fracture zone LD1 and from surface groundwaters. We estimate contaminant concentrations in groundwaters in LD1 in the geosphere model. We assume that contaminants in the surface groundwaters have the same concentrations, as estimated (in the biosphere model) for the water in the lake. The depth of the well is varied from 7.4 m to its maximum possible value of 200 m, and all other parameters are fixed at their median values. The symbol in the curve locates the position of the median value of the depth of the well.

at their median value. The figure shows that, for depths of the well greater than about 50 m, the volume of surface groundwater drawn into the well becomes zero, so that the well water demand is met entirely with deep groundwater moving upwards along LD1.

Because shallow wells draw less deep groundwater, they capture a smaller proportion of the contaminant plume. Figure D-45 shows the effect of the depth of the well on the fraction of the contaminant plume moving upwards in LD1 that is captured by the well (all other parameters are fixed at their median values). For overburden wells (those with a depth less than 7.4 m in the median-value simulation), only surface water is drawn into the well, thus the plume capture fraction is zero. For greater depths, the fraction captured increases because a greater proportion of groundwater is drawn into the well. The curve shows a maximum fraction of about 0.32 at depths of the well near 50 m, and the fraction decreases slightly to about 0.28 at a 200-m depth. This gradual reduction occurs because, at depths near 50 m, the well is most effective in focussing the groundwater flows, and thus the fraction of the plume captured is a maximum. At depths beyond 50 m, the well is slightly less effective in focussing groundwater flows; that is, there is a greater opportunity for deep groundwaters (and contaminants) to by-pass deeper wells.

- Well demand, or volume of water required by the well, is calculated in the biosphere model and depends on the number of persons making up the household of the critical group. This relationship is shown in Figure D-46. In the median-value simulation, the critical group uses this water to supply their domestic needs and to irrigate their garden. In general, well demand increases linearly with the size of the critical group because more water is required both for domestic purposes and for irrigation gardens. However, there is a limit on the well capacity, or the ability of the well to supply water; in the median-value simulation, it is 10 400 m^3/a. Water demand would exceed capacity if the size of the critical group were greater than 23 persons. Thus Figure D-46 shows a break in the curve between 23 and 24 persons. Beyond 23 persons, the well is used only as a source of domestic water, and thus well demand is significantly reduced. (Well capacity is affected by the depth of the well and groundwater velocity scaling factor: lower values of these parameters lead to smaller well capacities. These dependences are included in the figures described above; for example, in Figure D-43 the fraction of the contaminant plume in LD1, that is captured by the well, shows a maximum that is attributed to the effect of the groundwater velocity scaling factor on diminished well capacity.)

  Changes in well demand (dictated by the size of the critical group) also affect the fraction of contaminants captured by the well. This relationship is shown in Figure D-47. When the critical group consists of a single individual, the well demand is about 460 m^3/a, and approximately 0.11 of the contaminant plume moving up fracture zone LD1 is captured by the well. When there are 23 persons in the household of the critical group, the

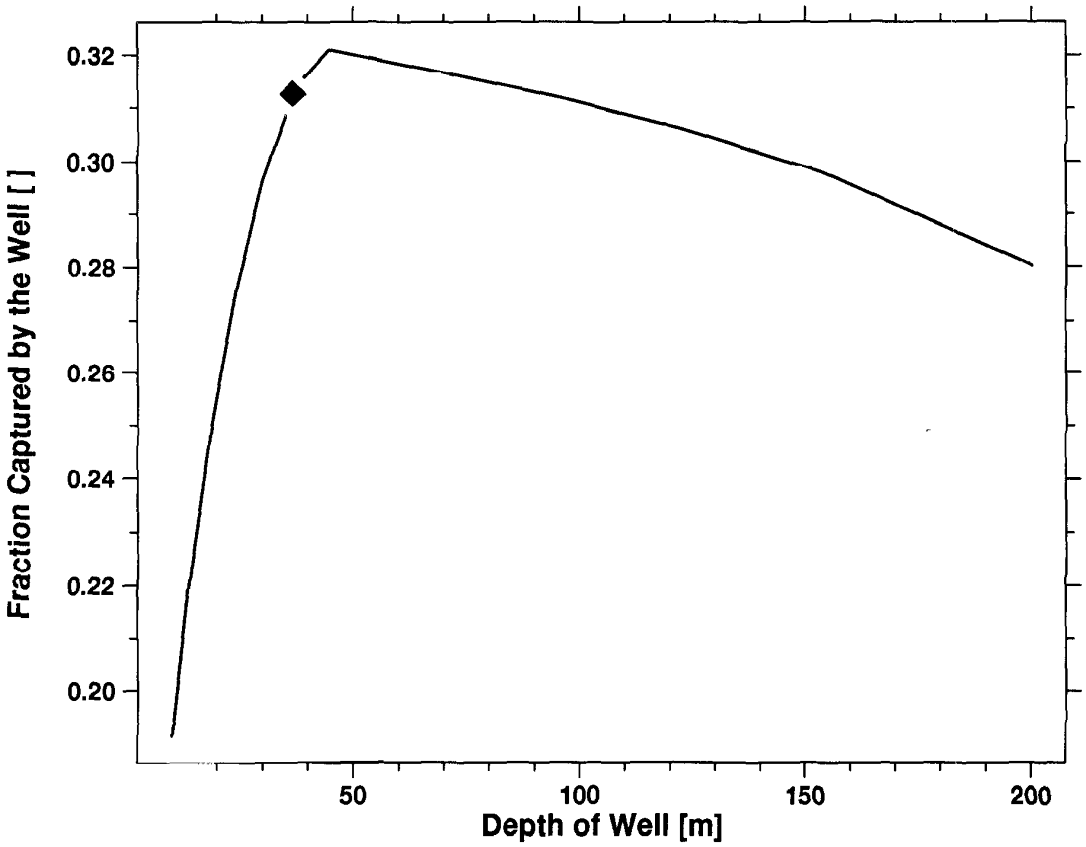

FIGURE D-45: Effect of the Depth of the Well on Contaminant Capture by the Well

The curve shows the effect of the depth of the well on the estimated fraction of the contaminant plume moving upwards in fracture zone LD1 that is then captured by the well (all other parameters are fixed at their median values). Wells less than 7.4 m deep (in the median-value simulation) do not intersect LD1 and do not draw contaminated groundwater from LD1. The maximum plume capture fraction occurs near a depth of the well of about 50 m and decreases slightly for greater depths because there is more opportunity for contaminants to by-pass deeper wells. The depth of the well is varied over its range of possible values; the symbol in the curve locates its median value.

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well demand is near well capacity, and the plume capture fraction reaches a maximum value of 0.94. For a larger-sized critical group, the capture fraction is smaller because the well supplies only domestic water. For example, when there are 24 persons in household of the critical group, well demand is reduced to 3600 m^3/a; the plume capture fraction, to 0.57.

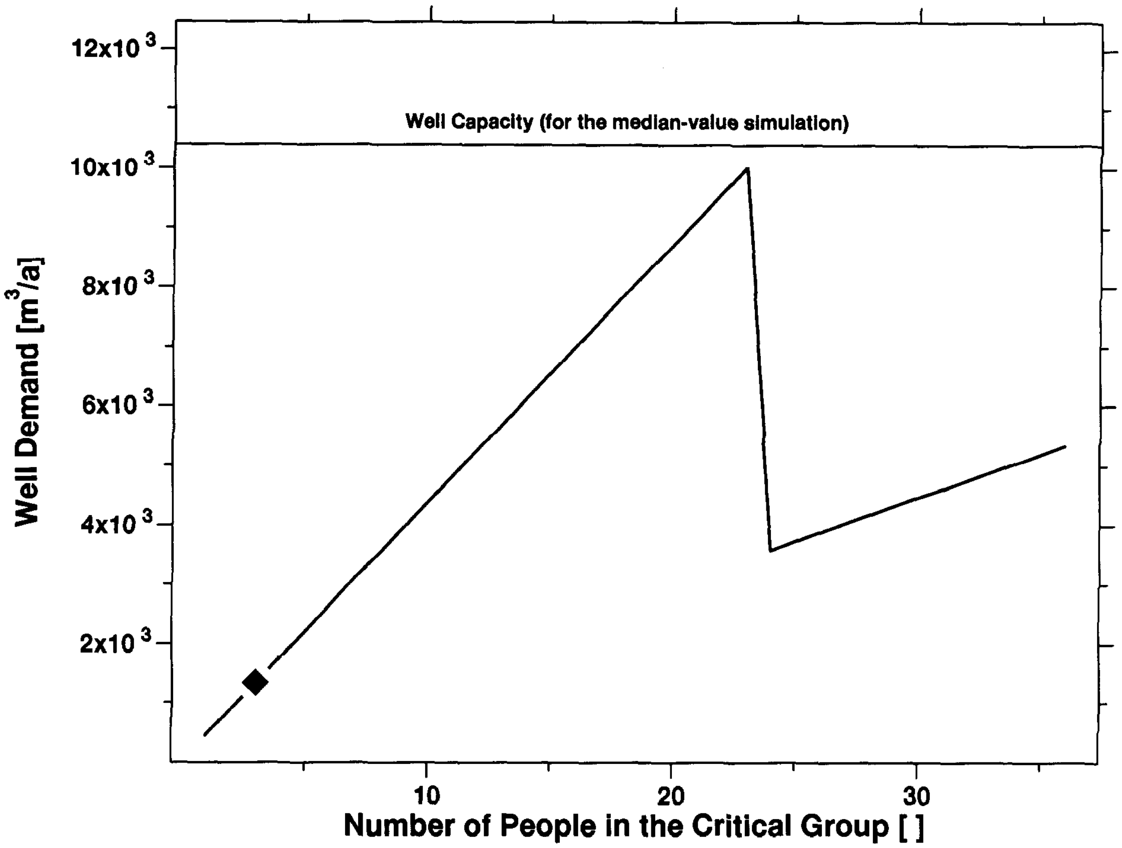

FIGURE D-46: Dependence of Well Demand on the Size of the Critical Group

Well demand refers to the volume of water withdrawn from the well and used by the critical group for domestic and irrigation purposes. The curve shows the effect of the number of persons making up the household of the critical group (size of the critical group) on estimated well demand when all other parameters are fixed at their median values. Well demand generally increases with the size of the critical group, but there is a break in the curve, between 23 and 24 persons, because water demand exceeds the well capacity to supply water (shown as a horizontal line at 10 400 m^3/a). For 24 or more persons, well water is used only for domestic purposes, thus well demand is reduced. The number of persons in the critical group is varied from 1 to 36; the symbol in the curve locates the value used in the median-value simulation.

D.7.3 EFFECTS OF THE GROUNDWATER VELOCITY SCALING FACTOR

The groundwater velocity scaling factor is used to increase or decrease groundwater velocities in all segments of the geosphere and is designed to reflect uncertainty in our knowledge of the groundwater flow system at the WRA (information from this area is used to construct the geosphere model). It is a multiplicative factor, with a median value of unity. The

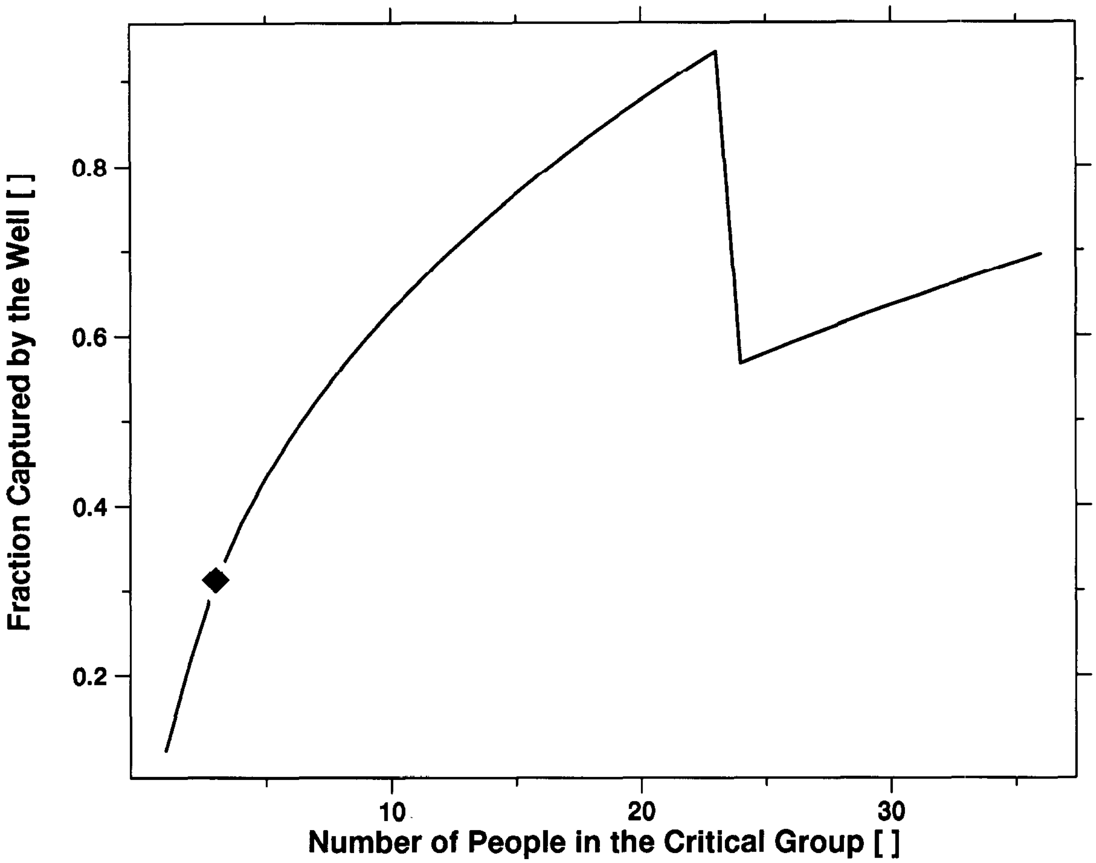

FIGURE D-47: Effect of the Size of the Critical Group on Contaminant Capture by the Well

The number of persons making up the household of the critical group (or size of the critical group) affects well demand, and thus the fraction of contaminants moving up fracture zone LD1 that is then captured by the well. The curve illustrates this relationship, where the number of persons is varied from 1 to 36; the symbol in the curve locates the value used in the median-value simulation. In general, the fraction captured increases with well demand, which follows the size of the critical group. The break in the curve between 23 and 24 persons reflects the change in well demand (Figure D-46).

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corresponding groundwater velocities in the median-value simulation then correspond to best estimates of groundwater movement for the conceptual hydrogeological model of the WRA. Permissible values of the groundwater velocity scaling factor range from 0.1 to 10, so that in any randomly sampled simulation the groundwater velocity in a segment is within 1 order of magnitude above or below its median velocity.

The discussion in the previous section suggests that the performance measure of the geosphere model is affected by the groundwater velocity scaling factor, which controls the amounts of contaminated and uncontaminated water that reach the well. Changes to the groundwater velocity scaling factor affect

- The drawdown of hydraulic heads caused by the well that influence groundwater flow velocities toward the well;

- The capture of contaminants by a well that is sufficiently deep to intersect fracture zone LD1 (Figure D-43);

- The release of contaminants from the vault through changes to the mass transfer coefficients (Section D.6.4); and

- The convective transport in moving groundwater of contaminants in all segments, including those within the waste exclusion distance (about 50 m of sparsely fractured rock between any vault room containing waste and fracture zone LD1).

For times up to 10^5 a, the two important discharge areas from the geosphere are the well and the South part of Boggy Creek (Section D.3). Figure D-48 shows the overall effect of the groundwater velocity scaling factor on total discharge of ^{129}I from the geosphere (at both the well and Boggy Creek South), whereas Figure D-49 shows the fraction of the total discharge that reaches the well. In general, total discharges of ^{129}I increase as a function of the groundwater velocity scaling factor, reflecting the increased convective transport of contaminants in the geosphere. However, the proportion discharged through the well decreases, showing a trend that is similar to the dependence on the groundwater velocity scaling factor of the fraction of the contaminant plume in LD1 captured by the well (compare Figures D-43 and D-49). The median value of the groundwater velocity scaling factor is 1.0, thus in the median-value simulation, about 30% of the total discharge of ^{129}I is to the well, and the remaining 70% is to Boggy Creek South.

Similar results are also observed for ^{14}C, except that the relatively short half-life of ^{14}C is an important factor. For example, discharges to Boggy Creek South involve additional delays during transport through the upper rock zone and overburden, and these delays are long enough so that radioactive decay significantly reduces ^{14}C discharge.

Figure D-50 shows the effect of the groundwater velocity scaling factor on the maximum ADE to 10^4 a. Although it is not shown in previous plots, the maximum ADE up to 10^4 a is almost entirely the result of ^{129}I discharges to the well. At this time, the ^{14}C and ^{129}I released from the vault are just beginning to be released from the geosphere for the median-value simulation. For values of the scaling factor smaller than about 4, contaminant transport is slow enough so that estimated releases from the geosphere and the ADEs are insignificant. Estimated releases and ADEs at 10^4 a become more important for values of the scaling factor larger than 4.

In general, estimated releases from the geosphere and the ADEs tend to increase at 10^4 a as the groundwater velocity scaling factor increases.

This trend changes somewhat at 10^5 a. Figure D-51 shows the effect of the groundwater velocity scaling factor on the maximum ADE to 10^5 a (^{129}I dominates the ADE up to this time). The curve is similar to that in Figure D-50 for large values of the scaling factor, but it displays a minimum and maximum near values of 0.24 and 2.4. An explanation of these results can be attributed to the effects discussed in previous figures:

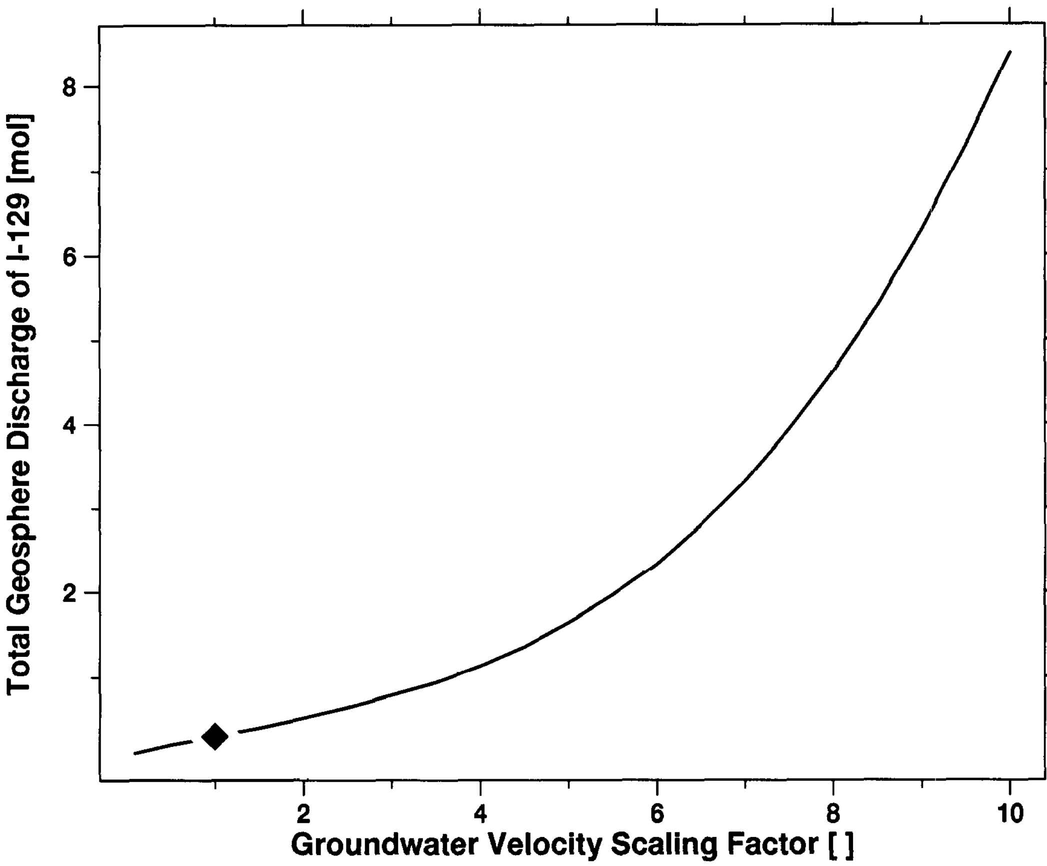

FIGURE D-48: Effect of the Groundwater Velocity Scaling Factor on Discharge of ^{129}I from the Geosphere

The curve shows the estimated total amount of ^{129}I released from the geosphere, up to 10^5 a, as a function of the groundwater velocity scaling factor (a dimensionless parameter) and when all other parameters are fixed at their median value. Over this time-scale, the contaminants are discharged only to the well and to Boggy Creek South. The groundwater velocity scaling factor is varied throughout the range defined by its PDF; the symbol in the curve locates its median value.

- For values of the groundwater velocity scaling factor above about 2.4, the fraction of total discharge to the well is relatively unchanged (Figure D-49), but the total discharge of ^{129}I shows a monotonic increase (Figure D-48). Therefore, the net discharge of ^{129}I to the well would also increase as the scaling factor increases beyond a value of 2.4. In the next section, it is noted that ADEs are greater for biosphere pathways involving the well than for pathways involving Boggy Creek South. Thus the maximum ADE also shows a monotonic increase (Figure D-51) related to the increased discharges of ^{129}I to the well.

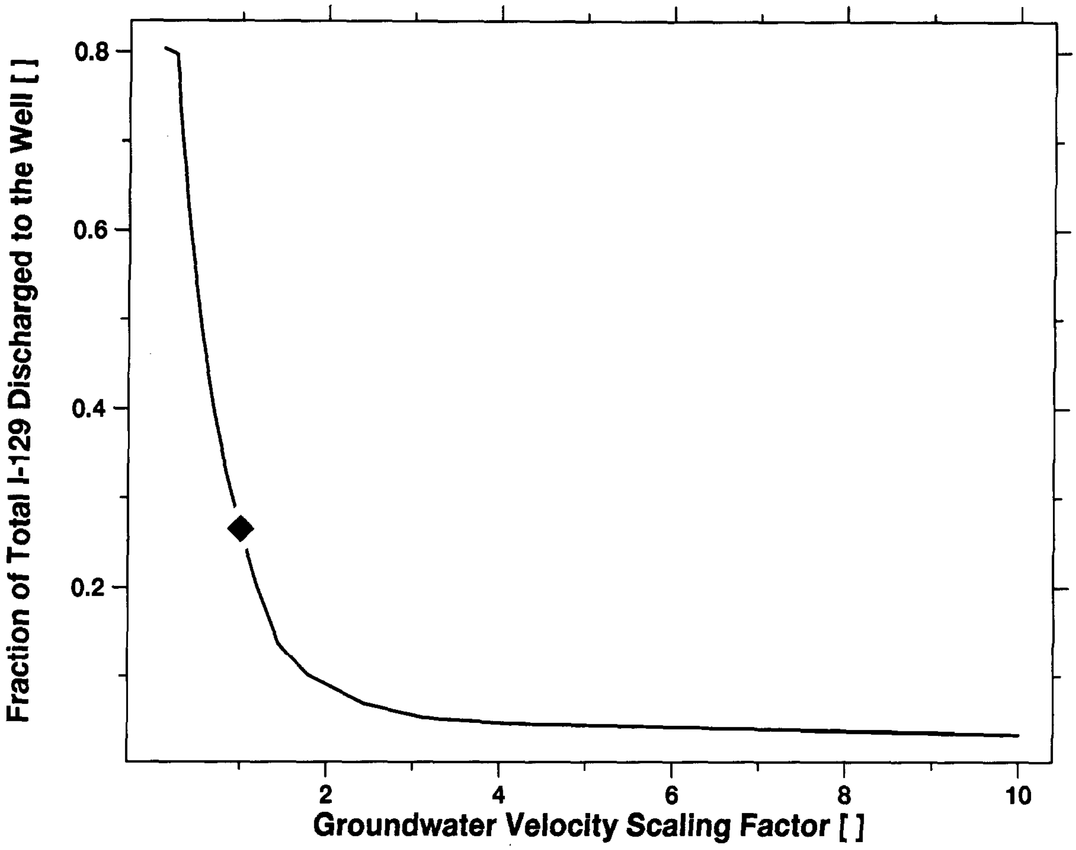

FIGURE D-49: Effect of the Groundwater Velocity Scaling Factor on ^{129}I Discharged to the Well

The vertical axis is the fraction of ^{129}I discharged to the well (or the estimated amount of ^{129}I discharged to the well divided by the estimated amount of ^{129}I discharged to the well and to Boggy Creek South), for times up to 10^5 a. The curve shows this fraction plotted as a function of the groundwater velocity scaling factor (a dimensionless parameter) and when all other parameters are fixed at their median value. Although the total discharge of ^{129}I increases as a function of the groundwater velocity scaling factor (Figure D-48), smaller fractions of the contaminant plume in LD1 are captured by the well (compare with Figure D-43).

- For values of the groundwater velocity scaling factor less than 2.4, the total discharge of ^{129}I is relatively small and unchanging (Figure D-48). However, greater fractions of this total discharge are captured by the well as the scaling factor is decreased from about 2.4 to 0.24. Therefore, the net discharge of ^{129}I to the well would also show an increase as the scaling factor is decreased over the same range. Thus, as before, the ADEs tend to increase as the groundwater velocity scaling factor is decreased from values near 2.4 to values near 0.24.

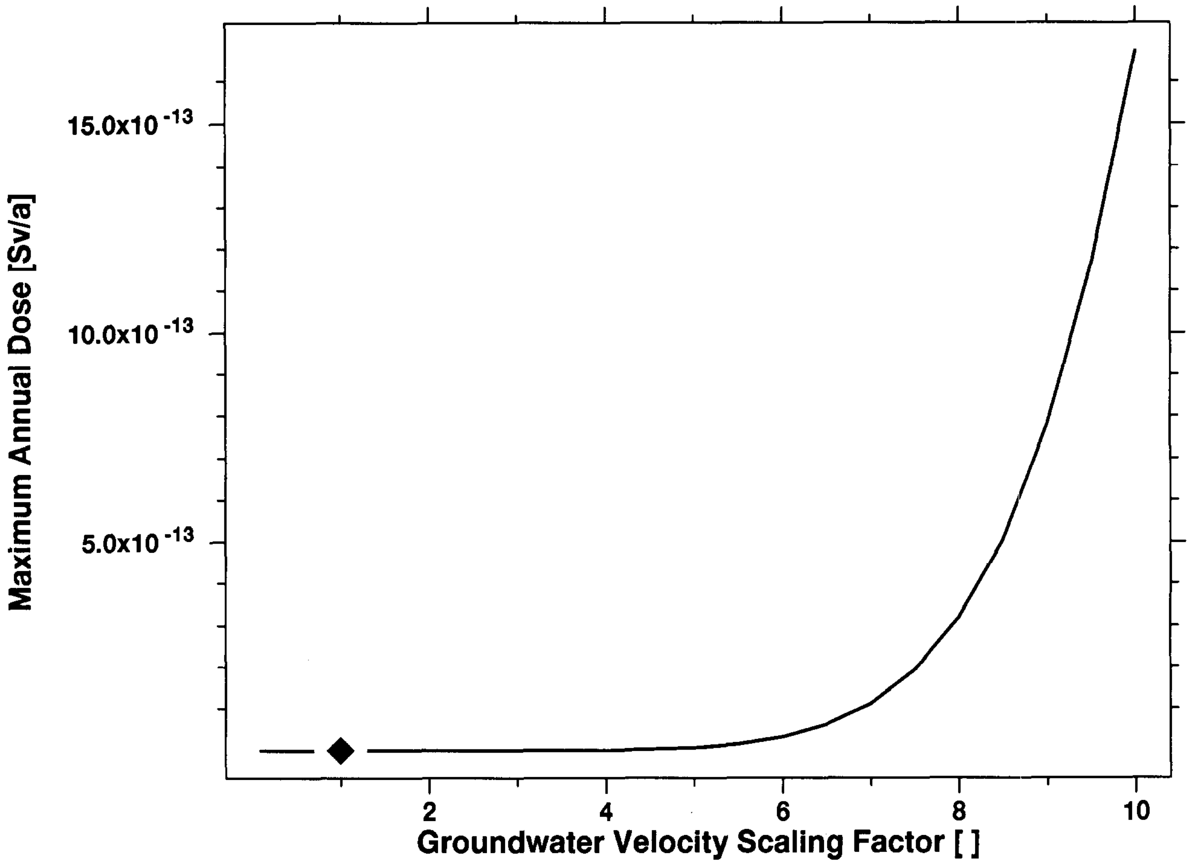

FIGURE D-50: Effect of the Groundwater Velocity Scaling Factor on Maximum Annual Dose to 10^4 a

The curve shows the maximum annual dose estimate (ADE) to 10^4 a as a function of the groundwater velocity scaling factor when all other parameters are fixed at their median value. Delays in the release and transport of contaminants are such that only ^{129}I and ^{14}C are beginning to be discharged at 10^4 a. Increases in the scaling factor correspond to decreases in delays resulting from transport in the geosphere, thus their rates of discharge (and the maximum ADE) increase. The groundwater velocity scaling factor (a dimensionless parameter) is varied throughout the range defined by its PDF; the symbol in the curve locates its median value at 1.0.

- Finally, as the groundwater velocity scaling factor is decreased below about 0.24, the fraction of the contaminant plume in LD1 captured by the well decreases (Figure D-43) in response to decreased well demand (the discussion in Section D.7.2 points out that when the scaling factor is less than 0.24, well demand must be reduced by drawing irrigation water from the lake, so that well demand would not exceed well capacity). Thus the ADE shows a parallel decrease.

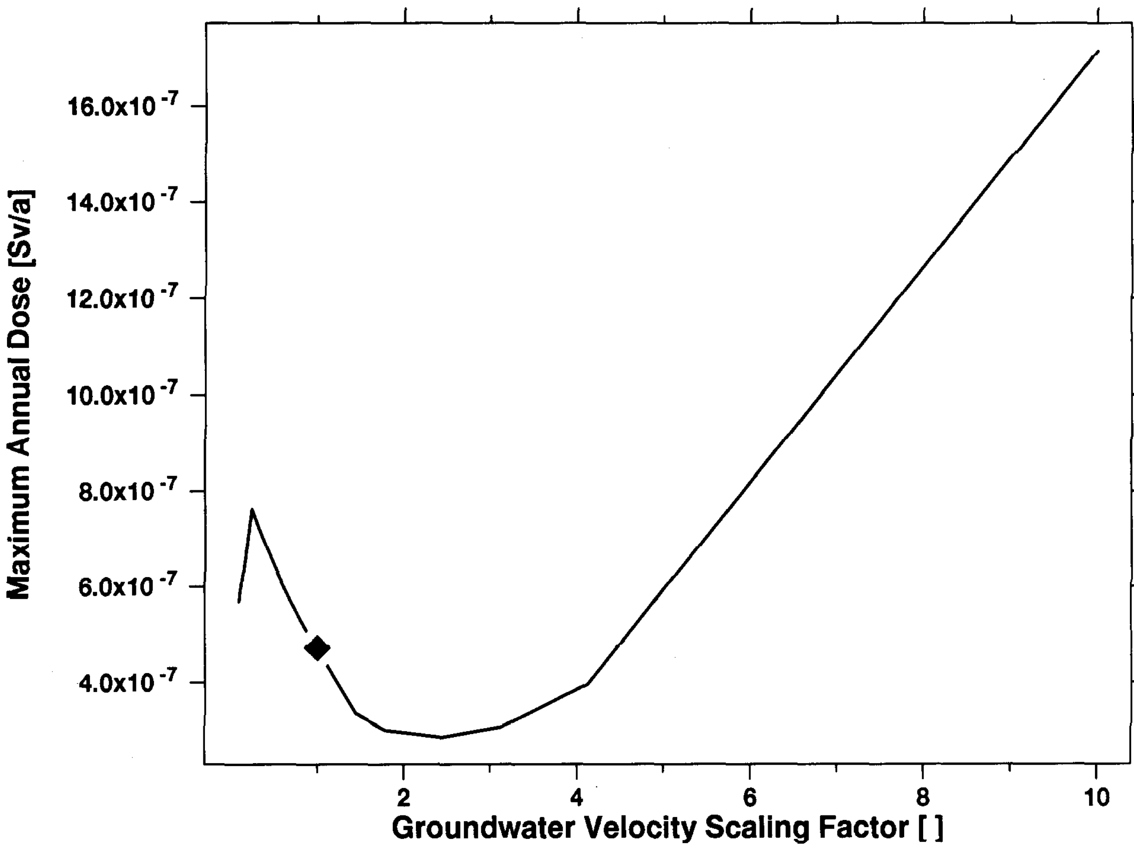

FIGURE D-51: Effect of the Groundwater Velocity Scaling Factor on Maximum Annual Dose to 10^5 a

Comments are as for Figure D-50, except that the maximum annual dose estimates are up to 10^5 a. The curve is more complex than that in Figure D-50 because of the effects of the groundwater velocity scaling factor on contaminant capture by the well and the well capacity (see text).

D.7.4 EFFECTS OF THE DEPTH OF THE WELL

The well is located such that it would intersect the centre line of the plume of contaminants that has been released from the vault and that is moving up fracture zone LD1. This centre line is not above the centre of the vault but skewed to the southwest corner because of the influence of the groundwater flow fields. The width of the contaminants plume is about 2000 m at the vault horizon, narrowing to about 1300 m at a depth of about 300 m. In the median-value simulation, the depth of the well is 37 m.

As noted previously, the depth of the well is one of three parameters that control the amounts of contaminated and uncontaminated water that reach the well. Changes to the depth of the well affect

- Whether the well is deep enough to intersect fracture zone LD1. We assume that wells with a depth greater than 7.4 m (in the median-value simulation) intercept LD1 and capture contaminated groundwater. Wells that are less deep capture only surface water, which is assumed to have the same concentrations of contaminants as does lake water.

- The relative proportions of uncontaminated surface water and contaminated deep groundwater drawn into the well (Figure D-44). Deeper wells tend to capture less surface water and more deep groundwater, thus providing less dilution of contaminants.

The results in Table 6-3 of the main text suggest that the depth of the well is an exceptionally important parameter for both ^{14}C and ^{129}I. However, the subsequent discussion in Section 6.3.3.3 shows its exceptional importance is actually an artifact of the full-range variation studies: the use of the smallest and largest well depths is similar to the use of the lake or a bedrock well respectively, as the source of domestic water (and thus the results are similar to those obtained for the switch that selects the source of domestic water).

In fact, the depth of the well is an important parameter, although not nearly as important as indicated in Table 6-3. To isolate the effects of the depth of the well, we limit the following analysis to a consideration of bedrock wells only. Thus the depth of the well is varied from 7.4 to 200 m.

Figures D-52 and D-53 illustrate the overall effect of the depth of the bedrock well, for times up to 10^5 a, on the total estimated discharges of ^{129}I to the well and the maximum ADE. Both figures show a pattern similar to that for the fraction of the plume in LD1 captured by the well (Figure D-45). The curves in both figures start at 7.4 m, the minimum possible depth of bedrock wells in the median-value simulation.

Inspection of Figures D-52 and D-53 shows that the total estimated discharges and the maximum ADE are attenuated for depths of the well less than 50 m. This variation is due to the effect of reduced plume capture and dilution of ^{129}I by surface water captured by the well, which becomes more important for wells less than about 50 m deep (Figure D-44). The maximum ADE is also slightly attenuated for depths of the well greater than about 50 m because of slight decreases in the fraction of the plume captured by the well.

Similar results are observed for ^{14}C except that the maximum ADE from ^{14}C shows a slight increase for depths of the well greater than 50 m. This effect occurs because there is less delay in transport of contaminants through the geosphere for deeper wells. For ^{14}C, which has a relatively short half-life, the effects of shorter delays (and lesser losses due to decay) outweigh the effects of slight decreases in the fraction of the plume captured by the well.

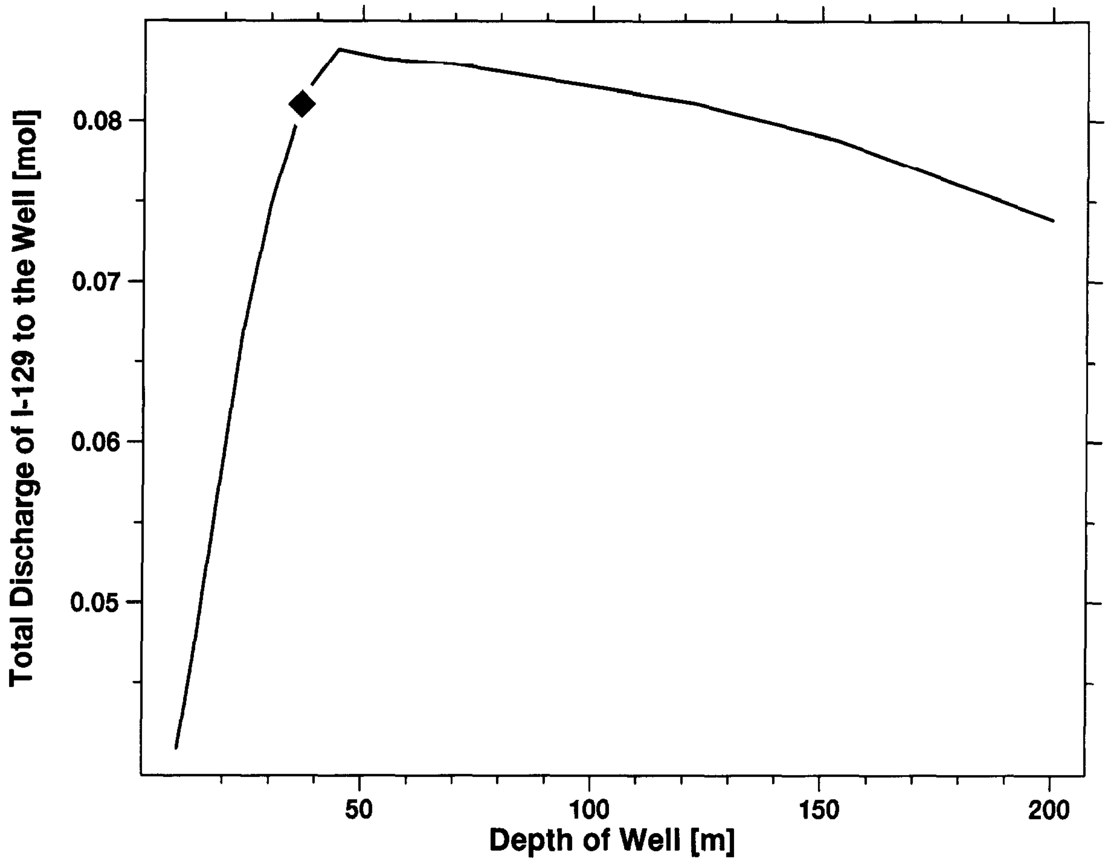

FIGURE D-52: Effect of the Depth of the Bedrock Well on ^{129}I Discharged to the Well

The vertical axis is the quantity of ^{129}I discharged to the well for times up to 10^5 a. The curve shows this quantity as a function of the depth of the well when all other parameters are fixed at their median value. The depth of the well is varied over its range of possible values; the symbol in the curve locates its median value of 37 m. The curve starts at a well depth of 7.4 m, which is the minimum depth of a bedrock well in the median-value simulation.

D.7.5 EFFECTS OF THE SIZE OF THE CRITICAL GROUP

The critical group consists of that group of individuals expected to be most exposed to contaminants from the reference disposal system. The critical group is assumed to be a sequence of self-sufficient rural households that lives its entire life at and obtains all its food, clothing, home furnishings, heating fuel and building materials from the area near the hypothetical disposal vault. The critical group also meets all its water requirements from local sources.

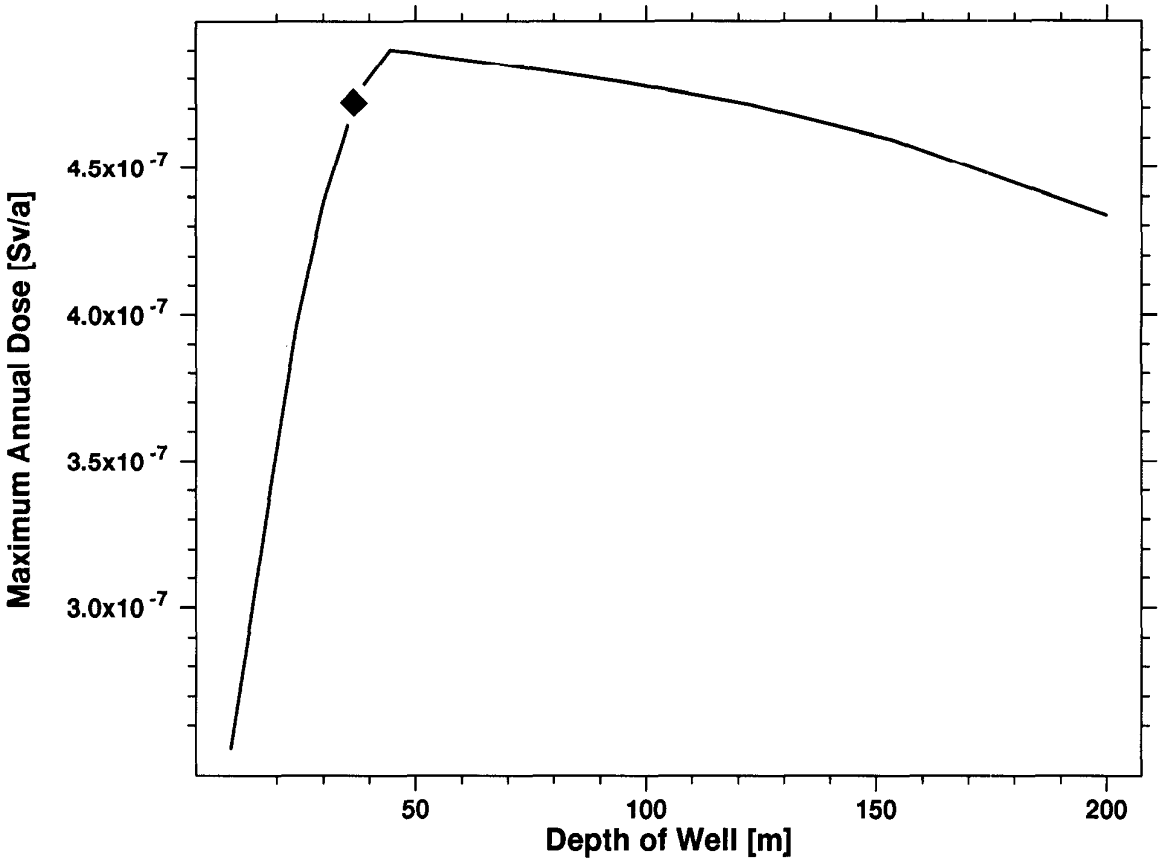

FIGURE D-53: Effect of the Depth of the Bedrock Well on the Maximum Estimated Annual Dose

The vertical axis is the maximum estimated annual dose up to 10^5 a. The curve shows this dose as a function of the depth of the well when all other parameters are fixed at their median value. The depth of the well is varied over its range of possible values; the symbol in the curve locates its median value of 37 m. The curve starts at a well depth of 7.4 m, which is the minimum depth of a bedrock well in the median-value simulation.

Changes to the size of the critical group affect the volume of water required from the well, or well demand, to satisfy domestic and irrigation purposes (Figure D-46). Changes to well demand, subsequently, affect the capture of contaminants by a well that is sufficiently deep to intersect fracture zone LD1 (Figure D-47).

Figure D-54 illustrates the overall effect of the size of the critical group, for times up to 10^5 a, on the maximum ADE (similar results are also observed for doses from ^{129}I or ^{14}C). The figure shows a break between 23 and 24 persons in the household of the critical group, resulting from

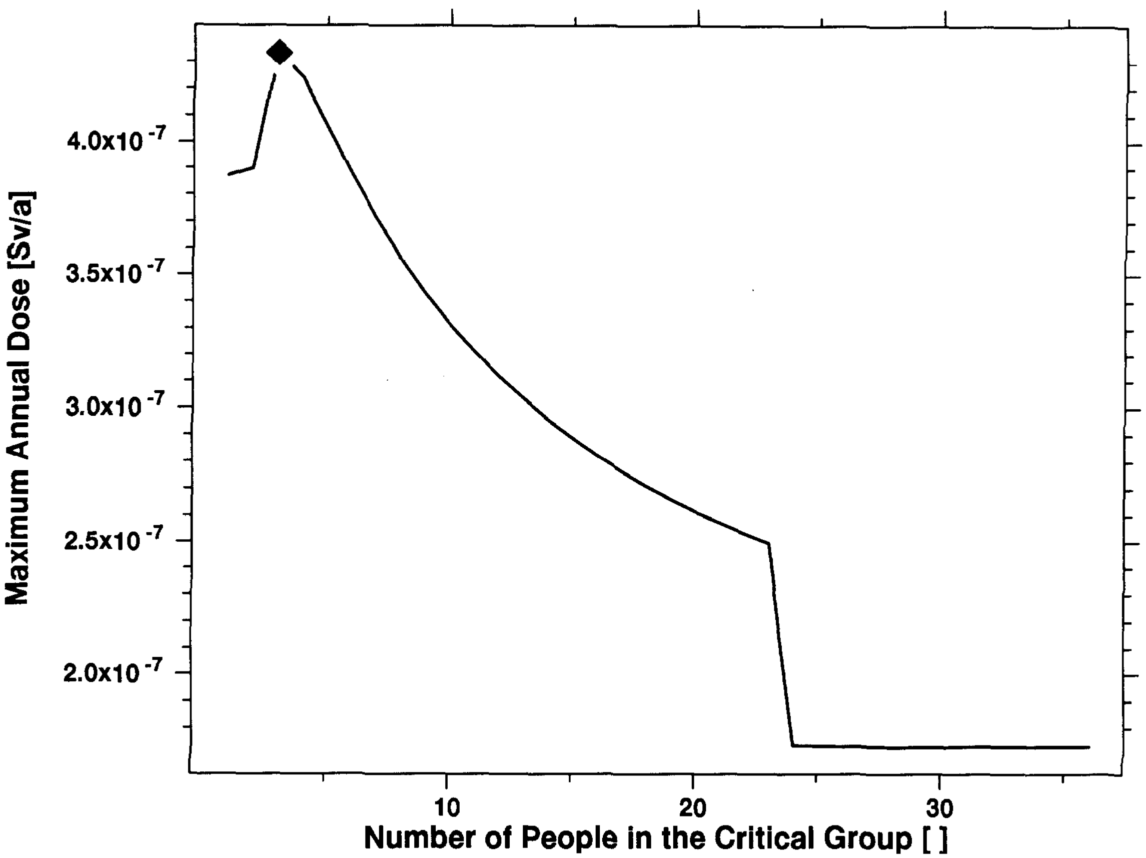

FIGURE D-54: Effect of Size of the Critical Group on the Maximum Estimated Annual Dose

The curve shows the maximum estimated annual dose up to 10^5 a as a function of the number of persons making up the household of the critical group (size of the critical group) and when all other parameters are fixed at their median value. The size of the critical group is varied from 1 to 36 persons; the symbol in the curve locates its median value of 3 persons. The complex nature of the curve is attributed to the combined effects of well capacity, well demand and fraction of ^{129}I captured by the well.

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changes in well demand (Figure D-46) and plume capture fraction (Figure D-47) that occur when well demand is reduced by drawing irrigation water from the lake so that well demand does not exceed well capacity.

The curve for the maximum ADE also shows a maximum at three persons and a general reduction as the number of persons in the household of the critical group increases. Both of these features are related to pathways in the biosphere model that are most important to radiation doses. In the median-value simulations, radiation doses are principally from pathways that involve well water (Section D.4):

- ingestion of ^{129}I in vegetables that were irrigated with water from the well, and

- ingestion of ^{129}I in drinking water from the well.

For both of these pathways, the ADEs would increase as concentrations of ^{129}I in well water increase.

In the median-value simulation, an increase in the size of the critical group leads to greater well demands (Figure D-46) and to greater capture by the well of ^{129}I moving upwards in LD1 (Figure D-47). However, the increases are not proportional. From Figures D-46 and D-47, as the size of the critical group doubles from 5 to 10

- the well demand increases by a factor of about 2, but

- the fraction of ^{129}I captured only increases by a factor of about 1.5.

In addition, other results show that the well demand is met with increasing proportions of diluting surface water. For example, doubling the size of the critical group from 5 to 10 persons increases the volume of surface water by a factor of about 5.

Thus concentrations of ^{129}I in well water actually decrease as the number of persons in the household of the critical group increases from 5 to 10 persons. This observation is illustrated in Figure D-55, which shows the maximum estimated concentration of ^{129}I in well water as a function of the size of the critical group. The maximum ADE (Figure D-54) shows a parallel decrease as the size of the critical group increases beyond about 3 persons. A similar effect was described by Reid et al. (1989).

The maximum in Figure D-54 occurs at three persons and, again, is attributed to estimated concentrations of ^{129}I in well water. (A plot of the maximum ADE from ^{129}I shows a maximum at three persons and, because ^{129}I dominates dose, Figure D-54 shows a maximum for the same number of people. A similar plot for ^{14}C shows a maximum at four persons, caused by the complicating effects of its relatively short half-life.) Inspection of Figures D-46 and D-47 show that, as the size of the critical group decreases from 3 to 1 persons, the fraction of contaminants captured by the well shows a greater proportional decrease than does the well demand; thus the concentration of ^{129}I also decreases. This decrease is evident in Figure D-55.

In the median-value simulation, the values of key parameters (affecting well demand, volume of surface water captured by the well and total amount of ^{129}I captured by the well) are such that ^{129}I concentrations in the well water and the maximum ADE reach a maximum when the size of the household of the critical group consists of three persons.

D.7.6 EFFECTS OF TORTUOSITY OF THE LOWER ROCK ZONE

Variations in the tortuosity of the lower rock zone have a large effect on both the maximum ADE to 10^5 a (Table 6-2 in the main text) and the geosphere performance measures (Table D-13). The geosphere model describes

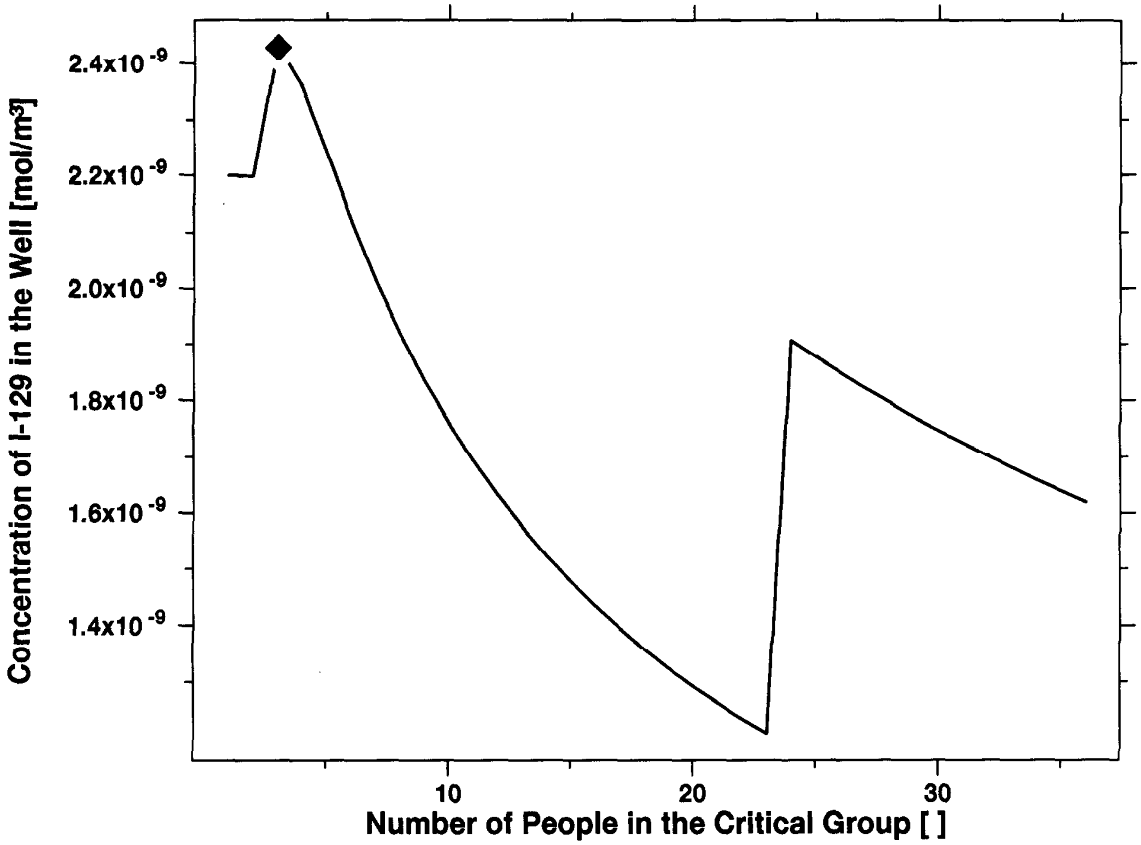

FIGURE D-55: Effect of Size of the Critical Group on ^{129}I Concentrations in the Well

The vertical axis is the maximum, up to 10^5 a, of the estimated concentration of ^{129}I in well water. The estimated concentrations are shown as a function of the number of persons making up the household of the critical group (size of the critical group) when all other parameters are fixed at their median value. The size of the critical group is varied from 1 to 36 persons; the symbol in the curve locates its median value of 3 persons. Note the similarity with the curve in Figure D-54.

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movement of contaminants by transport in moving groundwater (advection) and by diffusion. Diffusion is affected by the tortuosity of the medium, which is a measure of the increase in transport pathway caused by the tortuous nature of the water-filled spaces that contaminants follow during their movement. Delays in diffusive transport are (approximately) inversely proportional to the square of the tortuosity.

The effect of tortuosity is most significant in the lower rock zone immediately surrounding the vault (which includes rock within the waste exclusion distance). In this zone, groundwater velocities are small and contaminant transport is controlled by diffusion. (In other zones of the geosphere, groundwater velocities are much larger, and convective transport is more important.) Because diffusion is a relatively slow transport process and because the lower rock zone barrier is relatively large (the waste exclusion distance is about 50 m), the lower rock zone presents a major barrier to the transport of mobile contaminants, such as ^{129}I and ^{14}C.

Figure D-56 shows the effect of tortuosity on the total release of ^{129}I from the geosphere in 10^5 a. The maximum release occurs, as expected, for the minimum value of the tortuosity. This pattern also appears in Figure D-57, which shows the effect of tortuosity on the maximum ADE to 10^5 a. Similar results are also observed for ^{14}C, except that the curves drop more quickly as tortuosity increases, because radioactive decay of ^{14}C is more significant.

D.7.7 EFFECTS OF THE FREE-WATER DIFFUSION COEFFICIENT FOR IODINE

The free-water diffusion coefficient assigned to an element affects its rate of transport by diffusion in water, which is the process that dominates contaminant movement in the lower rock zone (including the rock within the waste exclusion distance).

The free-water diffusion coefficients for iodine and carbon were both identified as important parameters; the former is particularly important because ^{129}I is the largest contributor to the ADE up to 10^5 a. Figure D-58 shows the effect of the free-water diffusion coefficient for iodine on its releases from the geosphere in 10^5 a (similar results are observed for ^{14}C). The maximum release occurs, as expected, for the maximum value of the diffusion coefficient; a similar pattern also occurs in Figure D-59, which shows its effect on the maximum ADE to 10^5 a.

D.7.8 EFFECTS OF THE THICKNESS OF THE OVERBURDEN

As noted earlier, about 30% of the total discharge of ^{129}I is to the well, and the remaining 70% is to Boggy Creek South. If contaminants are discharged to Boggy Creek South instead of the well, they must pass through additional barriers before reaching the biosphere: the upper rock zone, a layer of overburden, and a layer of compacted lake sediment. The results in Table D-13 show that the thickness of the overburden has a small effect on the performance of the geosphere. (Note that the relative importance of the thickness of the overburden and related parameters, such as the thicknesses of the upper rock zone and lake sediment would increase for simulations that do not involve the well.) Both ^{129}I and ^{14}C are slightly sorbed onto minerals in overburden.

Figure D-60 shows the effects of changing the thickness of the overburden on the total estimated releases of ^{129}I from the geosphere, up to 10^5 a. Releases decrease as thickness of the overburden increases because of the additional delays in transport. Similar results are obtained for ^{14}C, except that releases are somewhat more attenuated as the thickness increases because of the relatively shorter half-life of ^{14}C.

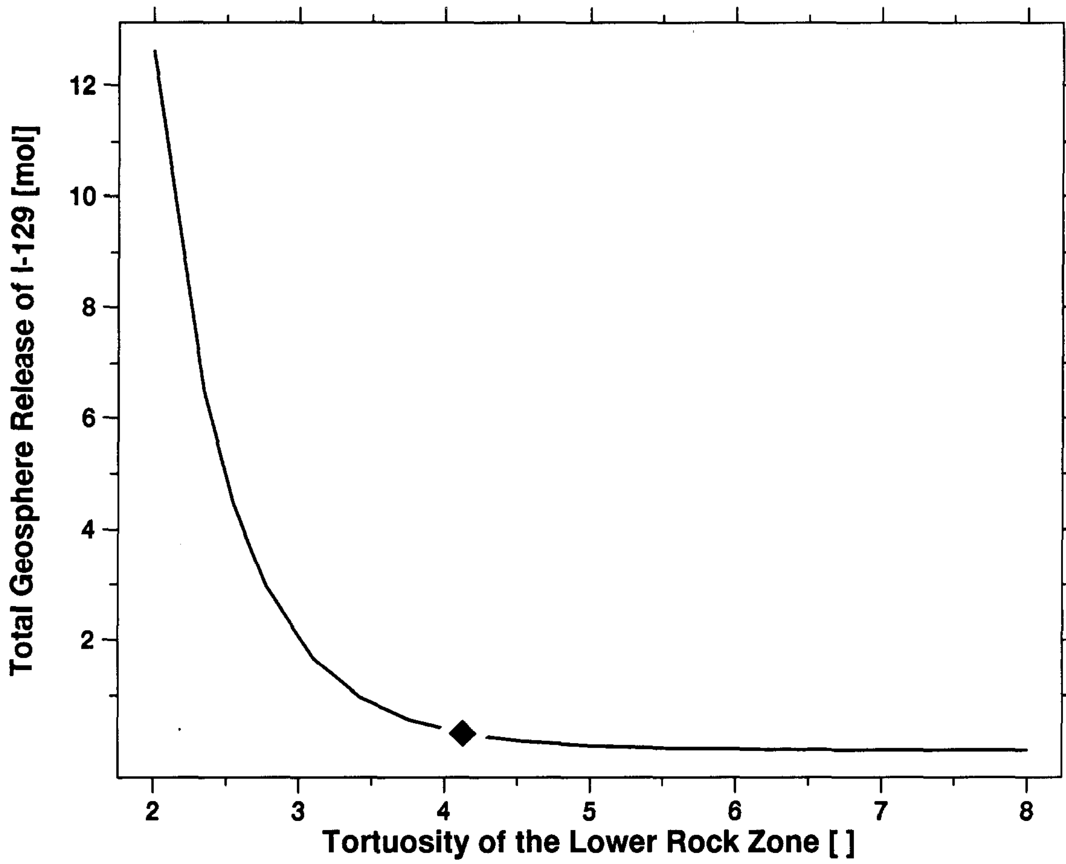

FIGURE D-56: Effect of Tortuosity on the Release of ^{129}I from the Geosphere

The curve shows the estimated amount of ^{129}I released from the geosphere in 10^5 a as a function of the tortuosity of the lower rock zone when all other parameters are fixed at their median value. Tortuosity (a dimensionless parameter) is a measure of the tortuous pathway that contaminants follow during their movement by diffusion: larger values of tortuosity correspond to effectively longer pathways and, therefore, longer delays in contaminant transport. The tortuosity is varied throughout the range defined by its PDF; the symbol in the curve locates its median value.

D.8 SENSITIVITY ANALYSIS OF THE BIOSPHERE MODEL

D.8.1 IMPORTANT PARAMETERS OF THE BIOSPHERE MODEL

One of the more important observations from the sensitivity analysis of the median-value simulation is that only two nuclides contribute significantly to maximum annual dose estimate (ADE) up to 10^5 a. They are ^{129}I and ^{14}C, with ^{129}I clearly dominating radiation doses at all times and for all combinations of parameter values. For this reason, sensitivity analysis of

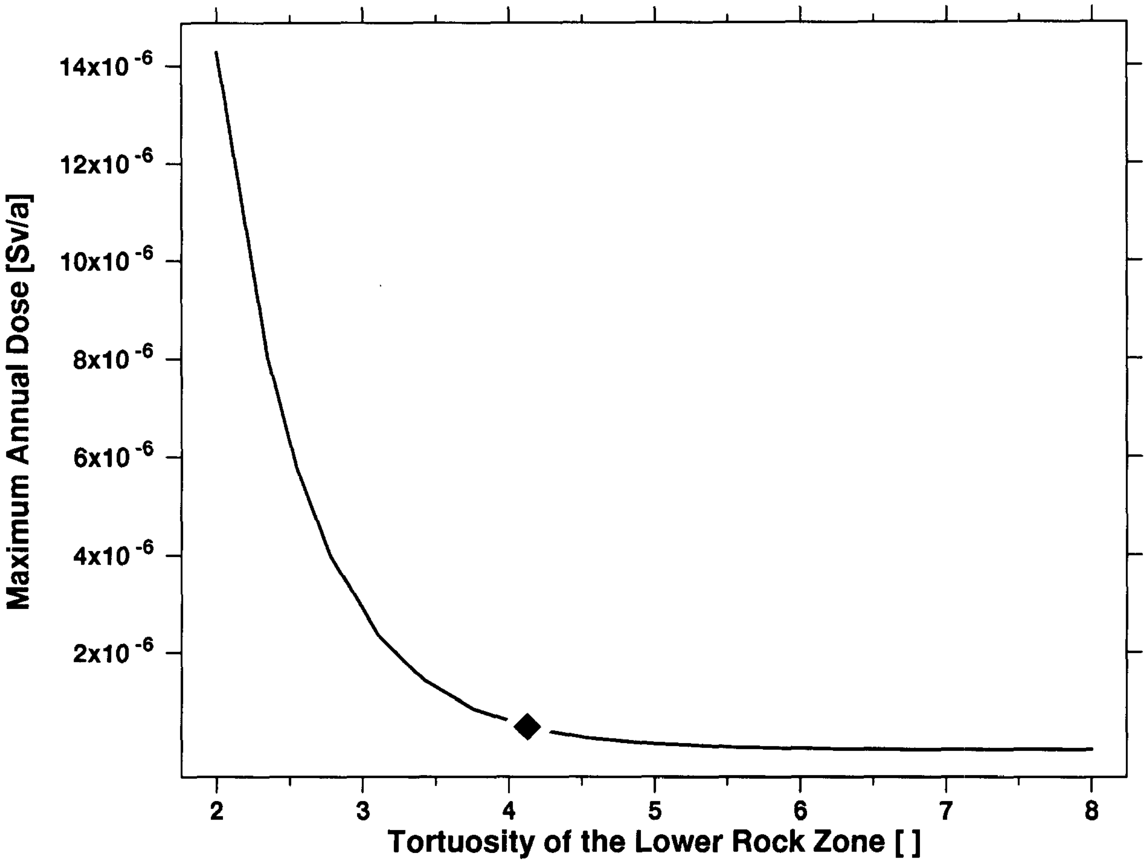

FIGURE D-57: Effect of Tortuosity on the Maximum Estimated Annual Dose

Comments are as for the previous figure, except that the vertical axis shows the maximum estimated annual dose up to 10^5 a.

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the biosphere model in the median-value simulation is focussed on these two nuclides. The results presented here are similar to those from the analysis of the biosphere model on its own (Davis et al. 1993). (Some results are not identical because our analysis deals with the total system model and includes the influence of the vault and geosphere models.)

The screening of parameters and features of the system model identified four important parameters used in the biosphere model (Table 6-2 in the main text):

- the plant/soil concentration ratio for iodine (a parameter describing the relationship between iodine concentrations in plants and in the soil on which they grow);

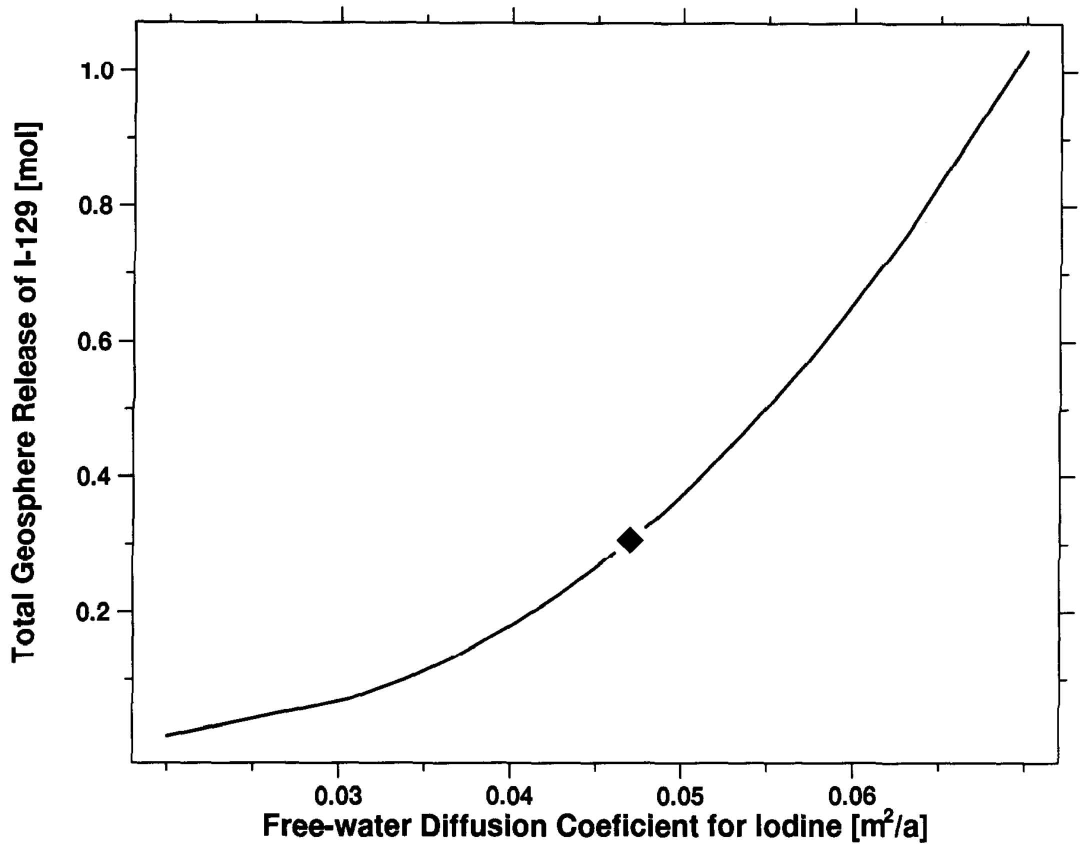

FIGURE D-58: Effect of the Free-Water Diffusion Coefficient for Iodine on ^{129}I Release from the Geosphere

The curve shows the estimated amount of ^{129}I released from the geosphere in 10^5 a as a function of the free-water diffusion coefficient for iodine when all other parameters are fixed at their median value. Iodine-129 releases are strongly affected by its rate of diffusive transport through the lower rock zone; lower diffusion coefficients correspond to lower rates of transport. The diffusion coefficient is varied throughout the range defined by its PDF; the symbol in the curve locates its median value.

- the iodine gaseous evasion rate (the rate constant describing the loss of iodine from soil by degassing);
- the carbon gaseous evasion rate (the rate constant describing the loss of carbon from soil by degassing); and
- the plant/soil concentration ratio for carbon.

These parameters are important in the median-value simulation in the sense that small variations of their values near their median values result in relatively significant changes to the maximum ADEs from ^{14}C or ^{129}I for times up to 10^5 a.

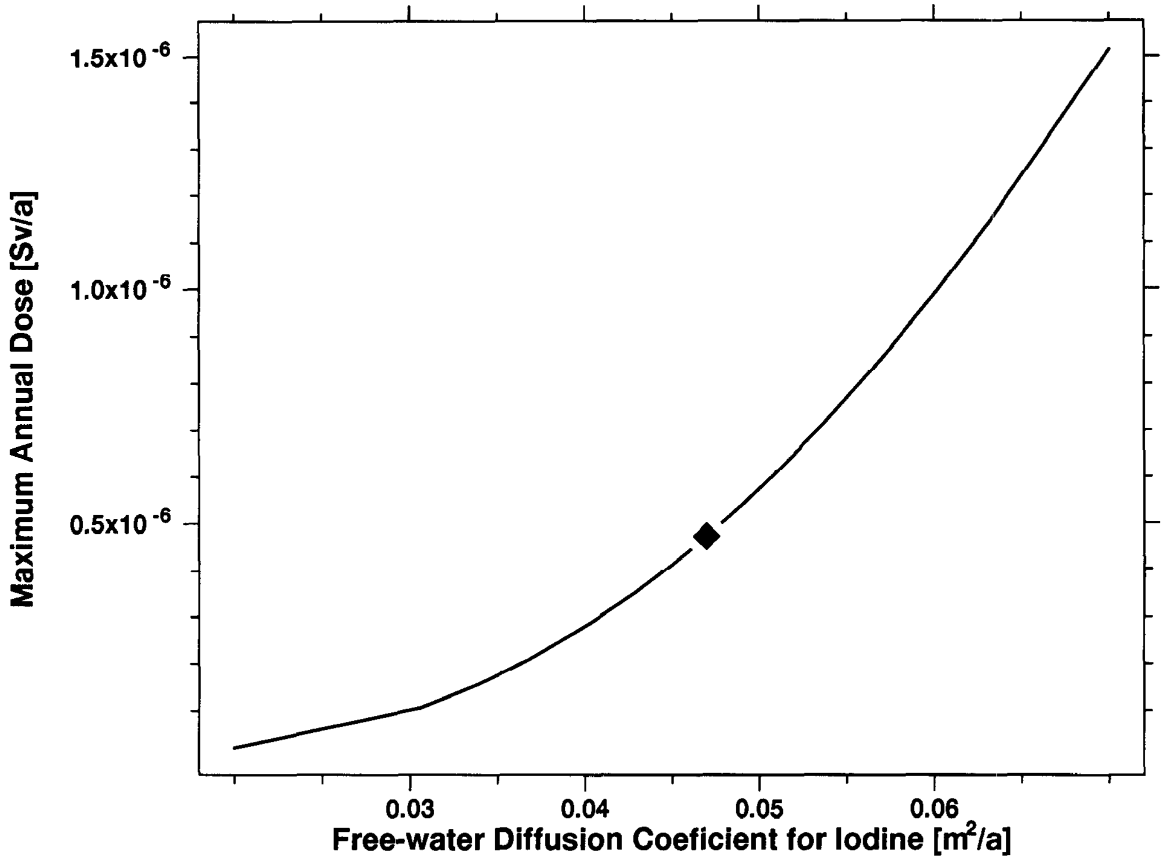

FIGURE D-59: Effect of the Free-Water Diffusion Coefficient for Iodine on the Maximum Estimated Annual Dose

Comments are as for the previous figure, except that the vertical axis shows the maximum estimated annual dose up to 10^5 a.

For variation of all sampled parameters (including the switch parameters) over their entire range of possible values, seven additional biosphere parameters are identified as important (Tables 6-3 and 6-4 in the main text). They are

- the aquatic mass loading coefficient for iodine (a parameter used to quantify the degassing of ^{129}I from the lake);

- the iodine plant environmental half-life (or residence time of iodine on plants);

- the number of persons in the critical group;

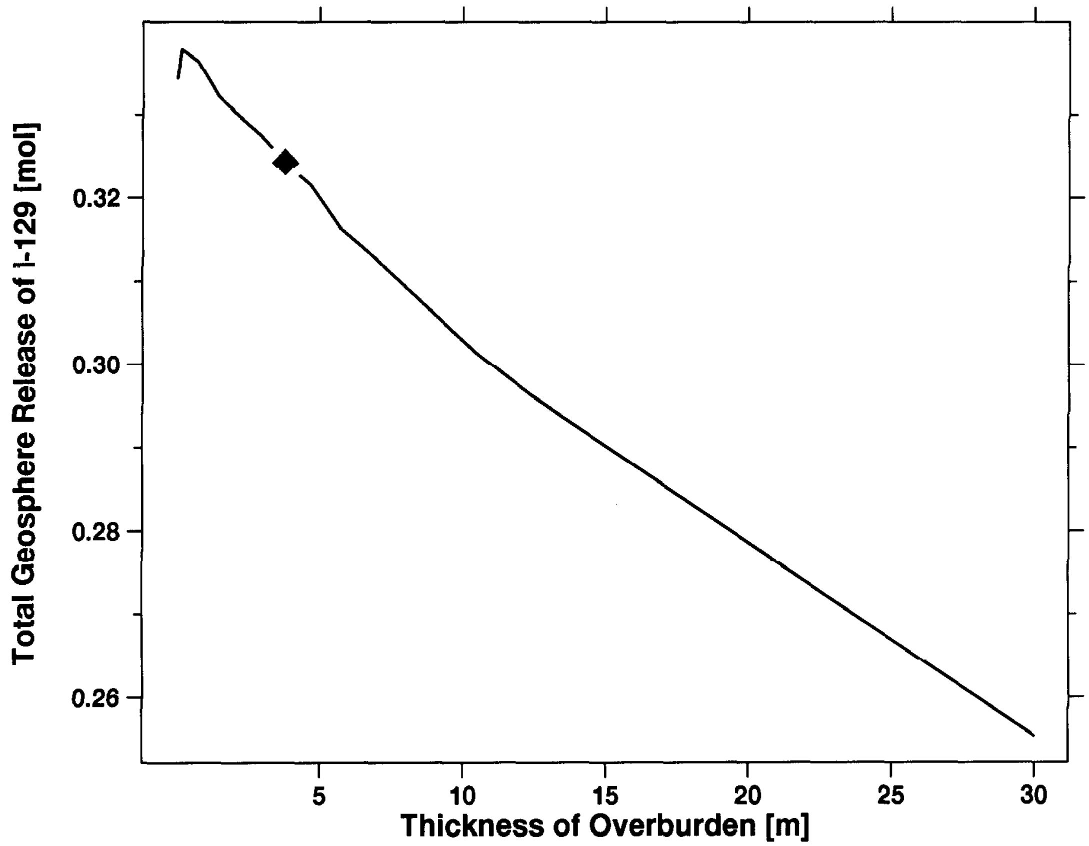

FIGURE D-60: Effect of the Thickness of the Overburden on Total Release of ^{129}I from the Geosphere

The curve shows the total estimated amount of ^{129}I released from the geosphere in 10^5 a as a function of the thickness of the overburden, which lies between the rock of the pluton and the surface. Increased thickness of the overburden results in greater delays in contaminant transport and smaller releases. Note that the overburden only affects discharges to Boggy Creek and the Pinawa Channel, and not discharges through the well. The thickness of the overburden is varied throughout the range defined by its PDF; the symbol in the curve locates its median value.

- the switch that selects lake water or well water as the source of domestic water (and, possibly, irrigation water) used by the critical group;

- the switch that selects whether the garden is irrigated;

- the switch that selects the type of soil in the garden, forage field, woodlot and peat bog; and

- the switch that selects fresh lake sediment as the soil in the garden, forage field, woodlot and peat bog.

A separate fractional factorial screening study was conducted on the biosphere model alone, examining the effects of system parameters on a measure of the performance of the biosphere. The biosphere performance measure for ^{129}I is defined as a ratio of integrals for times up to 10^5 a: the integral of the ADE from ^{129}I is divided by the total amount of ^{129}I that enters the biosphere. The performance measure represents the effectiveness of the biosphere in delaying transport of and attenuating impacts from ^{129}I: a greater value implies that the biosphere is less effective. Its units are Sv/mol. A similar performance measure is defined for ^{14}C.

This auxiliary screening identified as important the 11 parameters listed above and eight additional parameters:

- the plant-to-milk transfer coefficient for iodine;
- the fraction of human food energy derived from meat,
- the plant-to-poultry product transfer coefficient for iodine,
- the plant-to-mammalian meat transfer coefficient for iodine,
- the water-to-fish transfer coefficient for carbon,
- the plant-to-mammalian meat transfer coefficient for carbon,
- the plant-to-milk transfer coefficient for carbon, and
- the plant-to-poultry product transfer coefficient for carbon.

Table D-14 summarizes the dependence of the performance measure of the biosphere model on the 19 important parameters listed above. The relative effect of each parameter is shown by comparing the ratios in the table; for example,

- As was the case for the analysis of the vault and geosphere models, the relative importance of a parameter depends on whether the response examined is the maximum ADE (Tables 6-2 and 6-3 in the main text) or the biosphere performance measures (Table D-14).

- The source of domestic water has a strong effect on the performance measures for both ^{14}C and ^{129}I. As shown below, removing the well as a source of drinking water will decrease the maximum ADEs about 2 orders of magnitude.

- The type of soil in the fields used by the critical group also has a strong effect on both performance measures; whether or not the garden is irrigated has a smaller effect.

- Two parameters have a strong effect on the biosphere performance measure for ^{129}I only. They are the plant/soil concentration ratio for iodine and the gaseous evasion rate of iodine from soil. Similarly, the corresponding parameters for ^{14}C strongly affect only the ^{14}C performance measure.

TABLE D-14

RELATIVE IMPORTANCE OF PARAMETERS ON BIOSPHERE PERFORMANCE MEASURES*

Parameter	Ratios of Performance Measure for ^{129}I	^{14}C
Plant/soil concentration ratio for iodine	110	1.0
Source of domestic water	96	120
Soil type	20	5.8
Iodine gaseous evasion rate from soil	4.3	1.0
Irrigation of the garden	3.2	2.1
Number of persons per household	2.5	5.0
Iodine plant environmental half-life	2.0	1.0
Plant to milk transfer coefficient for iodine	1.6	1.0
Aquatic mass loading coefficient for iodine	1.5	1.0
Fraction of human food energy derived from meat	1.4	1.1
Plant-to-poultry product coefficient for iodine	1.3	1.0
Plant-to-mammalian meat coefficient for iodine	1.2	1.0
Fresh lake sediment used as soil	1.1	70
Carbon gaseous evasion rate from soil	1.0	53
Plant/soil concentration ratio for carbon	1.0	9.4
Water to fish transfer coefficient for carbon	1.0	2.8
Plant-to-mammalian meat coefficient for carbon	1.0	2.4
Plant-to-milk transfer coefficient for carbon	1.0	1.7
Plant-to-poultry product coefficient for carbon	1.0	1.5

* The parameters listed are those that have the greatest effect on measures of the performance of the biosphere. The performance measure for ^{129}I is defined as a ratio of two integrals calculated to 10^5 a: the integral of the estimated annual dose from ^{129}I divided by the integral giving the estimated amount of ^{129}I released from the geosphere. An equivalent performance measure is defined for ^{14}C. The two columns show ratios of the largest-to-smallest performance measures for ^{14}C and ^{129}I that are calculated when each parameter is separately varied over its range of possible values** and when all other parameters are fixed at their median values. A large ratio indicates that the parameter has a strong effect; a ratio of unity indicates that the parameter has no effect.

** For most parameters, the values actually used correspond to the 0.0, 0.02, 0.05, 0.1, 0.2, 0.3, 0.4, 0.51, 0.6, 0.7, 0.8, 0.9, 0.95, 0.98 and 1.0 quantiles. For some parameters, the 0.0 and 1.0 quantiles were excluded because their PDF are unbounded (as for "gaseous evasion rate from soil for iodine" and "plant/soil concentration ratio for iodine"). For "number of persons per household" (of the critical group), values used ranged from 1 to 36.

- Fresh lake sediment used as soil has a strong effect on the performance measure for ^{14}C but little effect for ^{129}I.

These observations are consistent with the results of the median-value simulation, discussed in Section D.4. For ^{129}I, the major pathways in the biosphere leading to the largest radiation doses, in decreasing order of importance to the maximum ADE to 10^5 a, are human consumption of

- plants contaminated through their roots and through their leaves by well water used to irrigate the garden,
- contaminated well water itself and
- milk and poultry products contaminated via well water given to the animals to drink.

The same pathways are important for ^{14}C, with the addition of meat consumption (principally contaminated by well water used as the source of drinking water for the animals) and fish caught in the lake.

In the following discussion, nine of the most important biosphere parameters listed above are discussed in two general groups. The first group, entitled "water and land use parameters", contains

- the switch selecting the source of domestic water (well or lake),
- the number of persons per household (of the critical group),
- the switch selecting whether the garden is irrigated,
- the switch selecting soil type, and
- the switch selecting use of fresh lake sediment as soil.

The second group is entitled "^{129}I and ^{14}C ingestion parameters", and contains

- the plant/soil concentration ratio for iodine,
- the iodine gaseous evasion rate from soil,
- the carbon gaseous evasion rate from soil, and
- the plant/soil concentration ratio for carbon.

The remaining 10 important biosphere parameters are not discussed further. They have a small effect on biosphere performance measures, and the reasons for the effects are relatively straightforward because they play a simple role in the biosphere model. For example, six describe the transfer of ^{14}C and ^{129}I from plants to milk, to mammalian meat and to poultry; all have a maximum effect of about 2.8, and they all behave similarly: greater values correspond to more contamination of food with ^{129}I or ^{14}C and, therefore, larger estimates of annual dose.

D.8.2 EFFECTS OF WATER AND LAND-USE PARAMETERS

Water and land-use parameters involve the size of the critical group and the switches that select their source of domestic water, the type of soil in their fields, whether they irrigate their garden and whether they use fresh lake sediment in their fields.

Table D-15 illustrates the effect of different options involving three of the four switches. The results show that

- For ^{129}I, the ADE up to 10^5 a is greatest when the well is used for drinking water and for irrigation of the garden. This option corresponds to the conditions selected for the median-value simulation.

- For ^{14}C, the greatest effect is observed when the well is the source of drinking water, the garden is not irrigated and lake sediment is used as soil. This option also leads to a slightly lower maximum ADE from the combination of ^{129}I and ^{14}C compared with the median-value simulation, principally because ^{129}I dominates the ADEs.

- Use of the lake instead of the well as the source of water reduces the maximum ADEs from both ^{129}I and ^{14}C by a factor of about 100.

- The maximum ADEs are somewhat smaller if the well is used only for drinking water compared with the option where it is used for both drinking and irrigation water.

- For ^{129}I, the time of the maximum ADE is 10^5 a for all options, reflecting the release of ^{129}I from the geosphere. (This time of maximum equals the end of the time period simulated in the median-value simulation; a global maximum would occur after about 10^6 a.)

- For ^{14}C, the times of the maximum ADE are near 6 x 10^4 a, largely paralleling releases from the geosphere that are strongly affected by radioactive decay (Section D.3). There are two reasons for the small differences in times of maxima between the options. The first reason is because of differences in transport paths in the geosphere: discharges at Boggy Creek South include additional delays in transport through the overburden and upper rock zone, and thus the time of maximum in option 2 of Table D-15 is slightly later than the time of maximum of option 1. The second reason is because of possible differences in time required for ^{14}C to reach maximum concentrations in well water and in garden soil. In the median-value simulation (or option 1 of Table D-15), well water and garden soil both reach maximum concentrations in 5.6 x 10^4 a (Section D.4), as do the resulting ADEs. In option 3 of the table, well water concentrations also reach a maximum at 5.6 x 10^4 a, but the buildup of ^{14}C in garden soil (from air deposition of ^{14}C released from the lake by gaseous evasion) occurs slightly later, such that the time of the maximum ADE is 5.8 x 10^4 a.

TABLE D-15

IMPORTANCE OF WATER AND LAND-USE SWITCHES IN THE BIOSPHERE MODEL*

Option and Description	Maximum Annual Dose Estimates (Sv/a) from: ^{129}I	^{14}C	Time of Maximum* for ^{14}C (a)
1. Well used for drinking water and for irrigation of garden	4.3×10^{-7}	3.8×10^{-11}	5.6×10^{4}
2. Lake used for drinking water and for irrigation of garden	4.4×10^{-9}	1.9×10^{-13}	6.7×10^{4}
3. Well used for drinking water and garden not irrigated	1.4×10^{-7}	1.3×10^{-11}	5.8×10^{4}
4. Well used for drinking water, garden not irrigated, and fresh sediment used as soil	3.9×10^{-7}	1.9×10^{-9}	6.6×10^{4}

* The results show the effects of choosing different options for land and water use assumed to be available to the critical group when all other parameters are fixed at their median values. The presence or absence of the well dominates the dose variation in the model. If a well is present, ^{129}I and ^{14}C doses are somewhat larger if the garden is irrigated. Locating a garden on fresh sediment leads to larger estimated ^{14}C doses than when the garden is on mature sandy soil, even if the soil is irrigated.

** For ^{129}I, the maximum ADE occur at 10^5 a in all cases.

Figure D-61 shows the effect of varying the switch that selects the well or the lake as the source of domestic water. The effects of this parameter cannot be shown as in previous plots where parameter values are varied because the switch has only two values: one selects well water and the other selects lake water. To illustrate its effect, we have taken data from a set of simulations in which all parameter values are sampled from their 0.475 and 0.525 quantiles. The figure confirms the importance of the well, and thus its corresponding switch, as a source of water used by the critical group.

This effect occurs for two reasons. The two important discharge locations within the 10^5-year time period are to the well (if present) and to Boggy Creek South, and

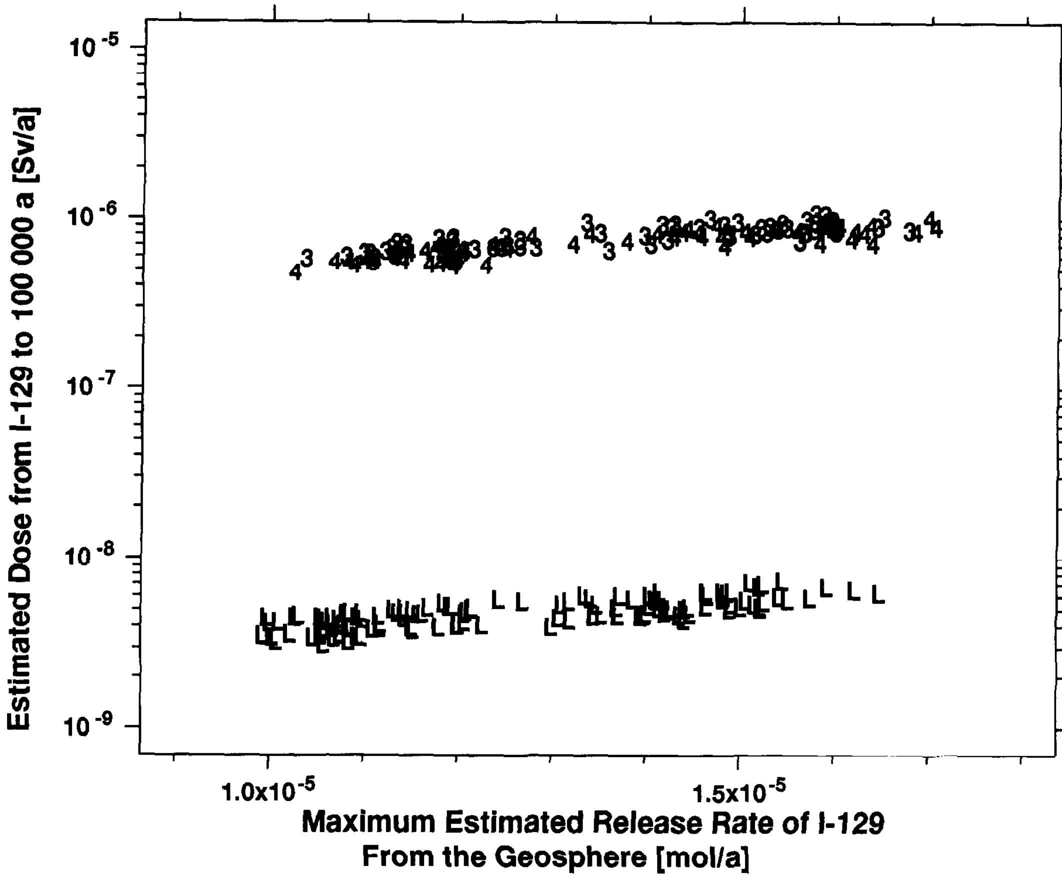

FIGURE D-61: Importance of Water and Land-Use Switches on Maximum Annual Dose Estimates to 10^5 a

The vertical axis is the maximum ADE for times up to 10^5 a and uses a logarithmic scale. The horizontal axis is the maximum estimated release rate of ^{129}I from the geosphere. The results are presented as a scatter plot; that is, each symbol represents one simulation and plots the maximum ADE from ^{129}I against the corresponding maximum estimated transport of ^{129}I from the geosphere. The results are taken from a set of simulations in which all sampled parameters have values near their median value (we used values corresponding to the 0.475 and 0.525 quantiles).
The symbols identify the source of water used by the critical group for domestic and irrigation purposes:

- "L" denotes the source of water is the lake;
- "3" and "4" denote the source of water is the well, and the number of persons in the household of the critical group is three or four.

It is clear that the maximum ADEs are greater when the source of water is the well.

- Discharges to well water tend to lead more directly to members of the critical group than do discharges to Boggy Creek South. In particular, well water is directly consumed as drinking water by members of the critical group and may be used to irrigate their garden.

- Contaminants discharged into well water undergo less dilution and delay in transport compared with discharges to Boggy Creek South. Discharges into Boggy Creek South lead to the lake and the bottom of the soil column. Contaminants entering the lake will undergo substantial dilution, whereas contaminants entering the soil column are delayed before they reach plants that might be consumed.

Figure D-61 also suggests that the maximum ADEs from well water tend to be slightly smaller for simulations involving four persons in the household of the critical group, compared with three persons. The discussion in Section D.7.5 has shown that there is a small decrease in the maximum ADE as the size of the critical group increases from three to four persons (see Figure D-54). The small decrease arises because ^{129}I concentrations are expected to decrease: the larger well demand is met with a proportionally greater capture of water than ^{129}I. These effects are discussed in more detail in Section D.7.5 and by Reid et al. (1989).

Option 2 in Table D-15 shows that, if lake water is used for domestic purposes and to irrigate the garden, the maximum ADEs from both ^{129}I and ^{14}C are significantly reduced. This is because concentrations of ^{129}I and ^{14}C are much lower in lake water than in well water, so that there is much less contamination of drinking water and garden produce. There is a greater reduction in the ADE doses from ^{14}C than from ^{129}I because of the greater influence of radioactive decay of ^{14}C during the transport of contaminants to Boggy Creek South.

Comparison of option 3 with option 1 shows the effect of irrigation of the garden: if the garden is not irrigated (option 3), the maximum ADEs from both ^{129}I and ^{14}C are reduced (and are mostly caused by drinking water from the well). This effect is due to changes in the food chain pathways of the critical group. In the median-value simulation, consumption of produce from the garden is an important element of the food chain. This pathway becomes much less important if irrigation is not practised because contamination of garden produce is largely caused by irrigation with well water. (The garden produce pathway is not entirely eliminated because garden soil is also contaminated by deposition of airborne contamination derived from the lake.)

Option 4 in Table D-15 shows that the maximum ADE is substantially increased for ^{14}C when fresh lake sediment is used as soil. The biosphere model assumes that fresh lake sediment is newly removed from the lake bed and is saturated with contaminated groundwater arising from the discharge at Boggy Creek South. The model also assumes that carbon degasses rapidly from soil. Although degassing of lake sediment would start once the sediment is exposed to air, this process is not included in the biosphere model. For the simulations studied here, estimated concentrations of ^{14}C are, therefore, much greater in sediment because degassing is modelled for soil but not for sediment. The net effect is larger estimates of maximum annual dose from ^{14}C

because the dominant food-chain pathway for ^{14}C involves uptake through plant roots. This uptake is proportional to concentrations of ^{14}C, which are much larger in fresh lake sediment than in mature soil (even if the mature soil is irrigated with well water).

For ^{129}I, the maximum ADE is slightly reduced when fresh lake sediment is used as soil. This effect occurs because the degassing of iodine from terrestrial soil is relatively small (about 0.5% of the gaseous evasion rate for carbon) and is compensated for by irrigation with well water. Thus for the simulations studied here, estimated concentrations of ^{129}I in sediment (option 4) are slightly smaller than estimated concentrations in soil (option 1). It follows that the ADEs from ^{129}I are also slightly smaller when fresh lake sediment is used as soil.

The effect of the fourth switch, which selects soil type, is shown in Table D-16. The fields providing food (and wood and peat) for the critical group may all lie on one of four types of soil: sand, loam, clay or organic. (Or, as discussed above, the soil may be freshly exposed lake sediment whose characteristics are similar to organic soil.) The table shows that organic soil gives the largest ADEs for both ^{14}C and ^{129}I. This occurs because both ^{14}C and ^{129}I more strongly sorb onto organic soil than other soils, and thus their concentrations are greatest in organic soil. The dominant food-chain pathway for ^{129}I involves uptake through plant roots, and for ^{14}C involves uptake through plant roots and respiration of CO_2. Because uptake is proportional to concentration, the ADEs are greatest when the soil type is organic.

D.8.3 EFFECTS OF ^{129}I AND ^{14}C INGESTION PARAMETERS

There are four important parameters in this group. Two are specific to the behaviour of iodine in the biosphere, and two are specific to the behaviour of carbon in the biosphere. For both elements, the parameters describe their movement from soil to plants (the plant/soil concentration ratios) and their release from soil through degassing (the gaseous evasion rates from soil). We discuss below the effects of these two parameters for ^{129}I; similar effects hold for ^{14}C.

The plant/soil concentration ratio and gaseous evasion rates from soil for iodine are important in the median-value simulation because they affect the major pathway in the biosphere between the well and the plant food ingested by the critical group: consumption of plants contaminated through their roots by well water used to irrigate the garden. The gaseous evasion rates from soil affects the retention of ^{129}I in soil that arrives in irrigation water, whereas the plant/soil concentration ratio affects the subsequent concentration of ^{129}I in plants.

The effects of these two parameters on the ADEs from ^{129}I are as follows:

- Increasing the plant/soil concentration ratio for iodine increases the ADE from ^{129}I. Figure D-62 shows the effect of changing this parameter on ADEs originating from the pathway involving ^{129}I transfer from soil to plants to man. The figure shows that the ADEs from this pathway increase proportionally with the plant/soil concentration ratio. The proportional relationship arises because

TABLE D-16

IMPORTANCE OF SOIL TYPE ON ANNUAL DOSE ESTIMATES FROM ^{14}C AND ^{129}I*

Soil Type	Maximum of the Annual Dose Estimate (Sv/a) Due to: ^{129}I	^{14}C
Sand	4.3×10^{-7}	3.8×10^{-11}
Loam	7.1×10^{-7}	4.7×10^{-11}
Clay	7.0×10^{-7}	5.5×10^{-11}
Organic	$12. \times 10^{-7}$	$32. \times 10^{-11}$

* The results are from simulations in which all parameters are fixed at their median value, except for the switch selecting soil type. This switch takes on values that select the four soil types in turn (in the median-value simulation, the soil type selected is sand).

larger ratios correspond to larger concentrations of ^{129}I in garden produce consumed by the critical group and, therefore, larger radiation doses.

- Increasing the iodine gaseous evasion rate for soil decreases the ADE from ^{129}I. Figure D-63 shows the effect of changing this parameter on ADEs from ^{129}I. For this parameter, greater values correspond to smaller amounts of ^{129}I that are retained in the soil. Thus lower concentrations of ^{129}I would be available in the soil to contaminate plants via their roots, leading to a smaller ADE from ^{129}I.

D.9 DETAILED DESCRIPTION OF THE ANALYSIS OF BARRIER EFFECTIVENESS

D.9.1 DISCUSSION OF BARRIER PERFORMANCE MEASURES

The analysis described in Section 6.4 in the main text examines the effectiveness of five engineered barriers:

- the titanium container, waste matrices, buffer, backfill and precipitation of technetium in the buffer;

and three natural barriers:

- the rock within the waste exclusion distance and two parts of fracture zone LD1.

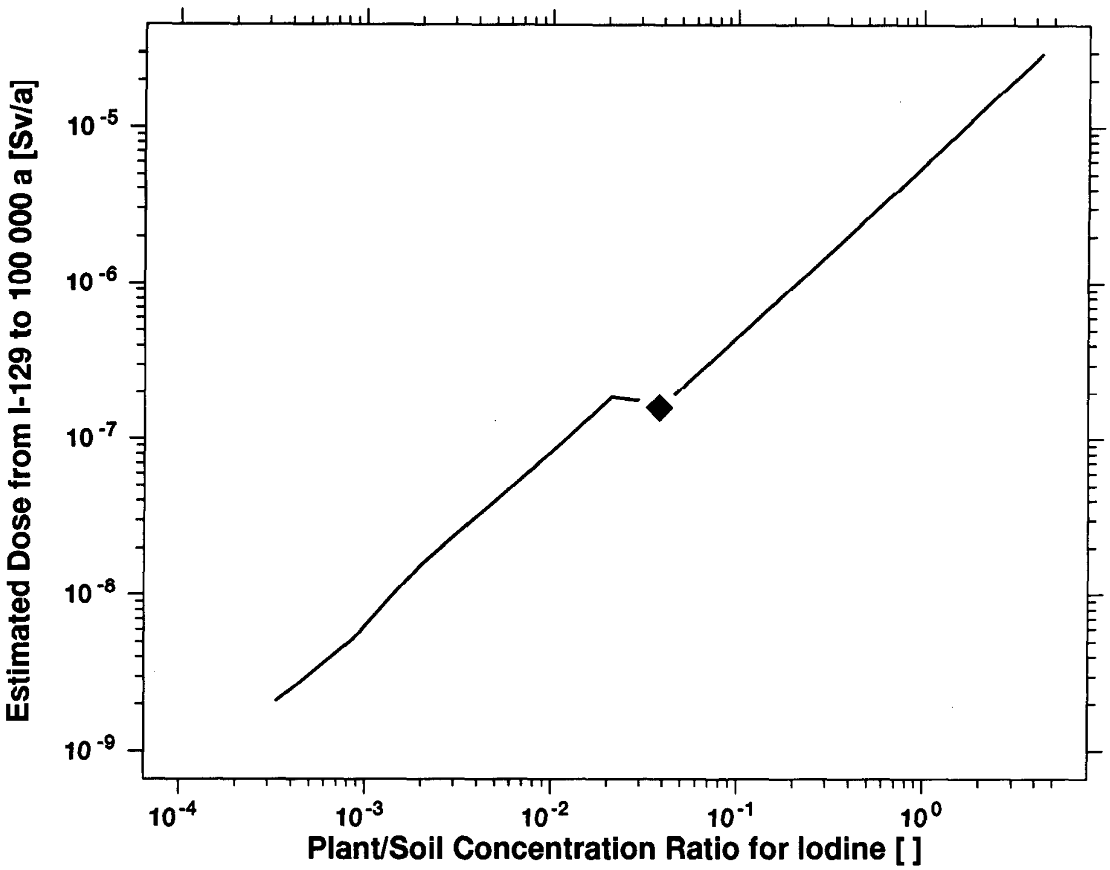

FIGURE D-62: Effect of the Iodine Plant/Soil Concentration Ratio

The vertical axis is the maximum, to 10^5 a, of the ADE from ^{129}I from the pathway involving ^{129}I transfer from soil to plants to humans (this ADE excludes all other pathways). The horizontal axis is the plant/soil concentration ratio for iodine, a parameter describing the transfer of ^{129}I from soil to plants. (The units of this parameter are shown as dimensionless; more accurately, they are Bq/kg wet biomass/Bq/kg dry soil.) Note that both axes use a logarithmic scale to cover the large ranges of values.

The plant/soil concentration ratio for iodine is varied over most of the range defined by its PDF (from the 0.05 to 0.95 quantiles), and the symbol in the curve locates its median value. All other parameters are fixed at their median value. Increasing the plant/soil concentration ratio corresponds to larger concentrations of ^{129}I in plants, and hence the ADE from this pathway increases. The discontinuity near the value of 0.05 is an artifact of the soil model (it uses two different mathematical algorithms, one on either side of the discontinuity, to calculate contamination buildup over different time-scales (Davis et al. 1993), and the algorithms do not match precisely).

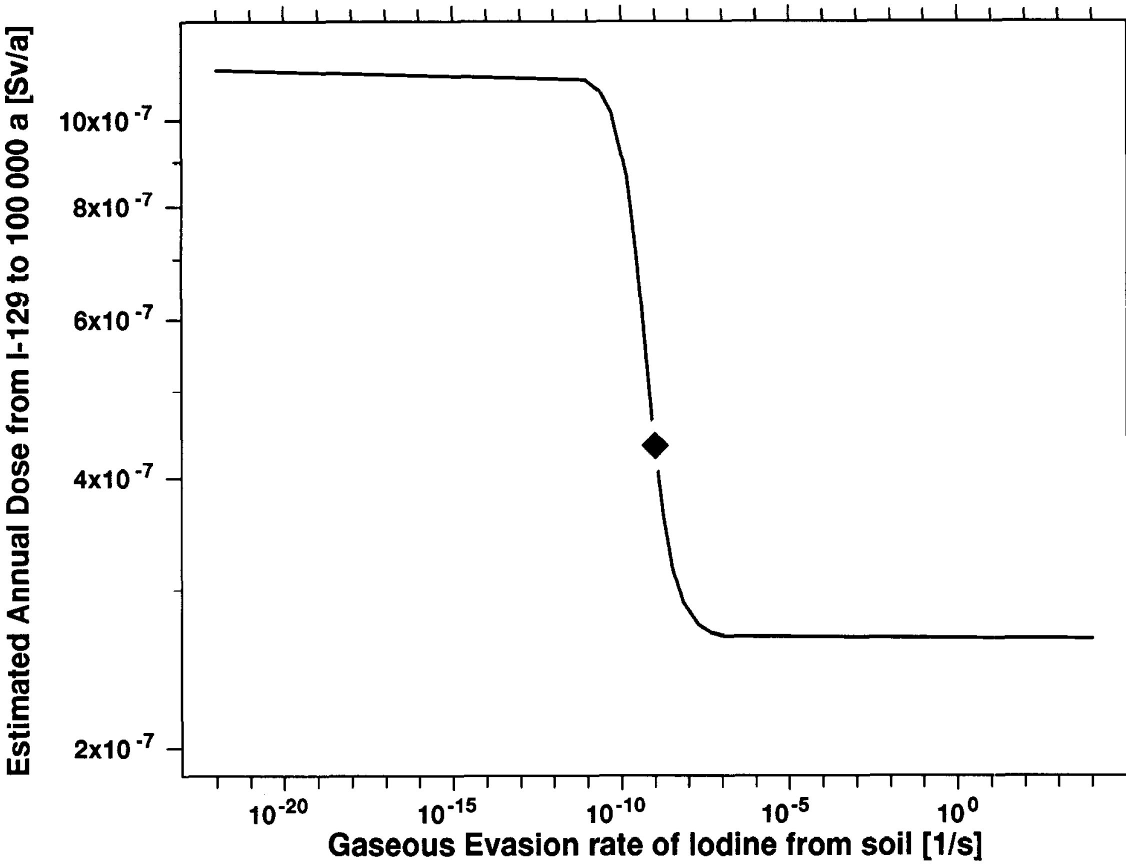

FIGURE D-63: Effect of the Iodine Gaseous Evasion Rate from Soil

The vertical axis is the maximum, to 10^5 a, of the ADE from ^{129}I from the pathway involving ^{129}I transfer from soil to plants to man. The curve shows how the maximum ADE changes as a function of the iodine gaseous evasion rate from soil when all other parameters are fixed at their median values. Note that both axes use a logarithmic scale to cover the large ranges of values.
The gaseous evasion rate is varied over most of the range defined by its PDF (from the 0.05 to 0.95 quantiles), and the symbol in the curve locates its median value. Increasing the iodine gaseous evasion rate corresponds to retaining smaller amounts of ^{129}I in soil, and thus the maximum ADE decreases.

(We classify precipitation as an engineered barrier because it occurs in the buffer and additives to the buffer could enhance precipitation. However precipitation may also be regarded as a natural barrier because it depends on the composition of groundwaters that enter the vault.)

To quantify the effectiveness of the barriers, we calculate a barrier performance measure for each contaminant. This measure has a simple definition:

$$\text{barrier performance measure} = \frac{\text{amount of contaminant exiting the barrier}}{\text{amount of contaminant entering the barrier}}.$$

Although the definition is simple, its application is not entirely straightforward, and we provide more details here on how the calculations are performed.

We follow a consistent mathematical method to calculate performance measures for each barrier: the method is equivalent to a "response" or Green's function approach for most barriers. That is, in most cases

- We assume that one unit of an amount of a contaminant enters the barrier instantaneously at time equal to zero; and

- We then calculate the total (integrated over time) amount that exits up to some following period of time, such as the next 10^4 a. These estimates use the models outlined in Sections 5.2 and 5.4 in the main text and the mathematical equations described in the primary references for the vault model (Johnson et al. 1994) and the geosphere model (Davison et al. 1994).

The barrier performance measure is then the ratio of the total amount that exits divided by the total (unit) amount that enters. This quantity is, therefore, a fraction representing the total amount (integrated over time) that passes through a barrier as a function of time.

Details for each of the barriers are as follows:

- Performance measures for the buffer, backfill, rock in the waste exclusion distance and the two parts of fracture zone LD1 are based on the response function method. LeNeveu (1987) describes response functions for the buffer and backfill; Heinrich and Andres (1985), for the geological media. These response functions include consideration of contaminant transport by moving groundwater, dispersion and diffusion, sorption and radioactive decay.

- The performance measure for the titanium containers is based on an equivalent approach. We assume a unit amount of contaminant is initially distributed evenly into all the containers in a vault sector. The container performance measure is then equal to the total fraction of the contaminant that is released as a function of time. We use the definition that a contaminant is completely "released" from a container at the instant of failure of the container. In reality, the instant of container failure corresponds to the earliest time that groundwater can begin entering the container. Contaminants are not completely released at this time, but they could (if the entire container were saturated) just be starting their slow diffusional movement from the container into the buffer. The fraction released is time-dependent because the containers fail at different times and because radioactive decay may modify the surviving inventory of a contaminant.

- The performance measure for the used-fuel matrix uses a modification to the response function method. We assume that all the titanium containers have failed at the start of the calculations.

Thus the entire mass of used fuel with all its contaminants is exposed to groundwater at time equal to zero. We then estimate the total amount of each contaminant that is released by the congruent- and instant-release mechanisms (Section 5.2 in the main text). It is the integral over time of the rate of release of the contaminant from the used-fuel into the buffer. The performance measure for the used-fuel matrix is this integrated amount released to the specified time divided by the initial inventory of the contaminant. From a pragmatic viewpoint, this method is equivalent to the response function method, because division by the initial inventory can be regarded as a correction that normalizes the input to the barrier to a unit amount.

- The performance measure for the Zircaloy waste matrix is calculated in the same manner as for the used-fuel matrix. Only the congruent-release mechanism applies to the Zircaloy matrix (Section 5.2 in the main text).

- The performance measure for the precipitation barrier is based on a different method. Many elements are relatively insoluble, and the vault model simulates their possible precipitation within the buffer (Section 5.2 in the main text). When precipitation occurs, the release of a contaminant will be attenuated (compared with its release from the waste matrix); typically, the attenuated releases will occur for a long time, until any accumulated precipitate has entirely re-dissolved. The effectiveness of this barrier depends in a nonlinear way on the rate of arrival of the contaminant. For example, precipitation would be most effective if the entire amount arrives at some instant in time and less effective if the arrival is distributed over a long period of time. This nonlinear behaviour means that the response function method cannot be directly applied to the precipitation barrier.

  To provide a reasonable estimate of the performance measure for the precipitation barrier, we include the effects of the prior barriers (waste matrices and containers) in estimating the amount that arrives at the precipitate. We then calculate the total amount that leaves the precipitate: it is the integral over time of the rate of release of the contaminant from the precipitate into the buffer. The performance measure for the precipitate barrier is then the total amount that leaves the precipitate divided by the total amount that arrives at the precipitate.

If radioactive decay is ignored, each barrier will eventually release all the contaminant, and thus the barrier performance measures will approach unity if the times considered are sufficiently long. Radioactive decay can result in values that range from zero to greater than unity:

- For most radionuclides, the amount that exits will be less than the amount that enters so that the performance measures will be less than unity. If a barrier is extremely effective, the measure will be zero.

- For some radionuclides, the decay of precursors may result in significant ingrowth, and the potential exit amount may be greater than the entrance amount. The corresponding performance measure would then be greater than unity.

- For all contaminants, the barrier performance measures will increase as a function of time, from an initial value of zero. The maximum possible value for the performance measures is unity for most contaminants and greater than unity only if ingrowth is significant.

Ingrowth is important only for radionuclides that are intermediate or end members of decay chains. They include members of the four actinide decay chains, such as ^{234}U (whose precursor is ^{238}U), and members of short decay chains, such as ^{32}P (from ^{32}Si). Section 5.9 in the main text identifies these radionuclides. We do not consider ingrowth in the analysis of barrier effectiveness but instead examine the effects of the barriers on each radionuclide in turn. We also do not consider radionuclides that are assumed to be in secular equilibrium with their precursors, because the movement of these radionuclides is simulated only in the biosphere model.

Figures D-64 to D-66 show some performance measures, or total fractions released, as a function of time for ^{14}C, ^{99}Tc and ^{238}U (Figure 6-12 shows similar curves for ^{129}I). The performance measures are both nuclide-dependent and time-dependent.

Figure D-64 summarizes the results for ^{14}C. It shows that

- The rock within the 50-m waste exclusion distance is clearly the most effective barrier. It significantly delays the release of ^{14}C: the total fraction released is less than 10^{-5} for about 2.5×10^4 a. The rock in the waste exclusion distance also attenuates releases; for example, the total fraction released never exceeds about 10^{-4}. This bound is a result of the radioactive decay of ^{14}C (with a half-life of 5730 a). In fact, the total fraction released for many barriers is significantly less than unity because of the effects of radioactive decay.

- The backfill is somewhat less effective, with a maximum of less than 10^{-2} in the total fraction released.

- The maximum in the total fraction released from the waste matrix (used fuel) is less than 10^{-1}. That is, less than 10% of the initial inventory of ^{14}C would leave the used-fuel waste matrix. This value is consistent with two considerations: releases of ^{14}C from used fuel are almost entirely due to its instant-release fraction (13% in the median-value simulation), and radioactive decay of ^{14}C significantly reduces its inventory before it diffuses from the waste matrix into the buffer. (The used-fuel matrix would be even more effective as a barrier for ^{14}C using the recent data described by Johnson et al. (1994) for the instant-release fraction of ^{14}C.)

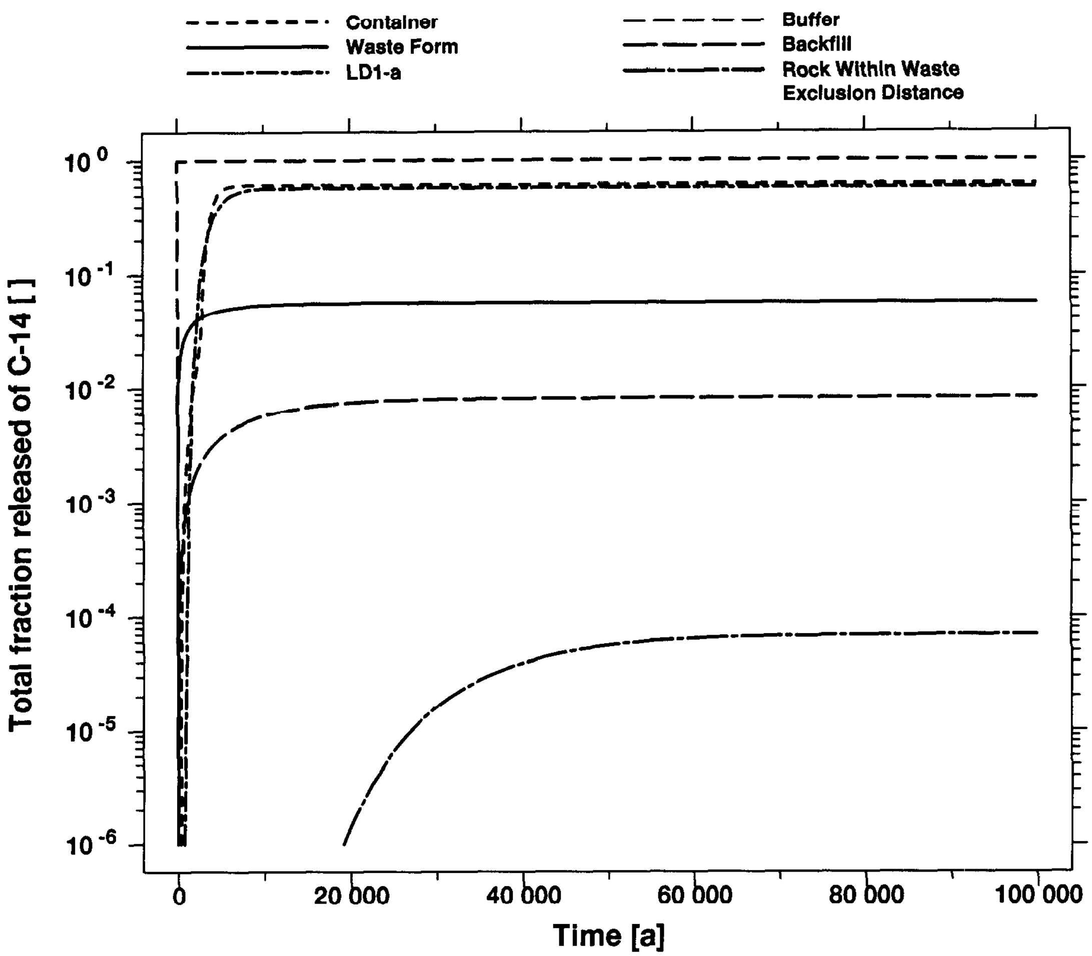

FIGURE D-64: Barrier Performance Measures for ^{14}C from Used Fuel

These six curves are calculated from the models for six barriers: used-fuel waste matrix, container, buffer, backfill, rock within the waste exclusion distance and the lower part (LD1-a) of fracture zone LD1. The curves show the fraction released from each barrier as a function of time; this assumes a known amount of ^{14}C is instantaneously input to the barrier at time equal to zero. The vertical axis plots the total fraction released from the barrier (or the performance measure of the barrier for ^{14}C). The most effective barrier for ^{14}C is the rock within the 50-m waste exclusion distance. The next most effective barriers are the backfill and used-fuel waste form.

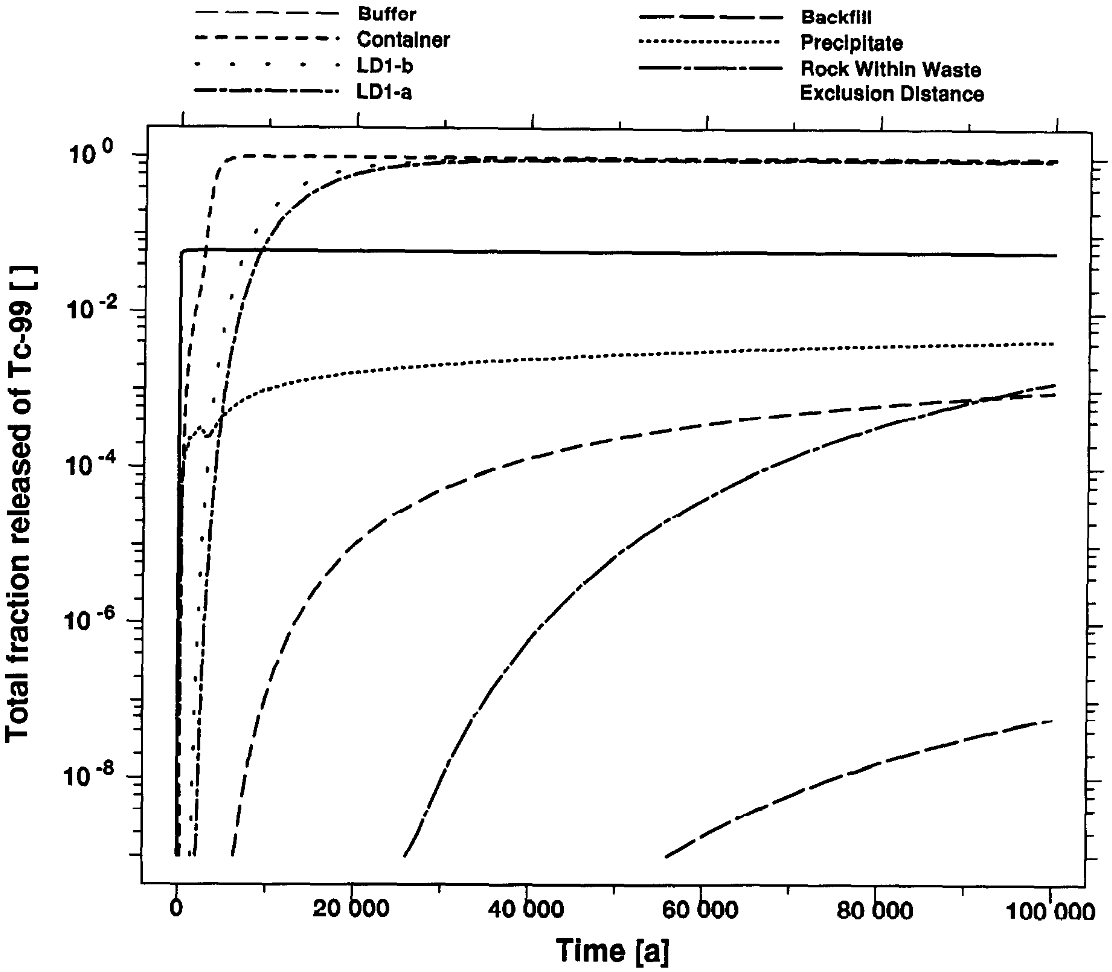

FIGURE D-65: Barrier Performance Measures for ^{99}Tc from Used Fuel

These eight curves are calculated from the models for the eight barriers: used-fuel waste matrix, container, buffer, backfill, rock within the waste exclusion distance and the lower (LD1-a) and upper (LD1-b) parts of fracture zone LD1, and precipitation. This last barrier describes the effects of precipitation of ^{99}Tc within the buffer. The curves show the fraction released from each barrier as a function of time; this assumes a known amount of ^{99}Tc is instantaneously input to the barrier at time equal to zero (except for the precipitation barrier; see text). The vertical axis plots the total fraction released from the barrier (or the performance measure of the barrier for ^{99}Tc).
The most effective barrier for ^{99}Tc is the backfill.

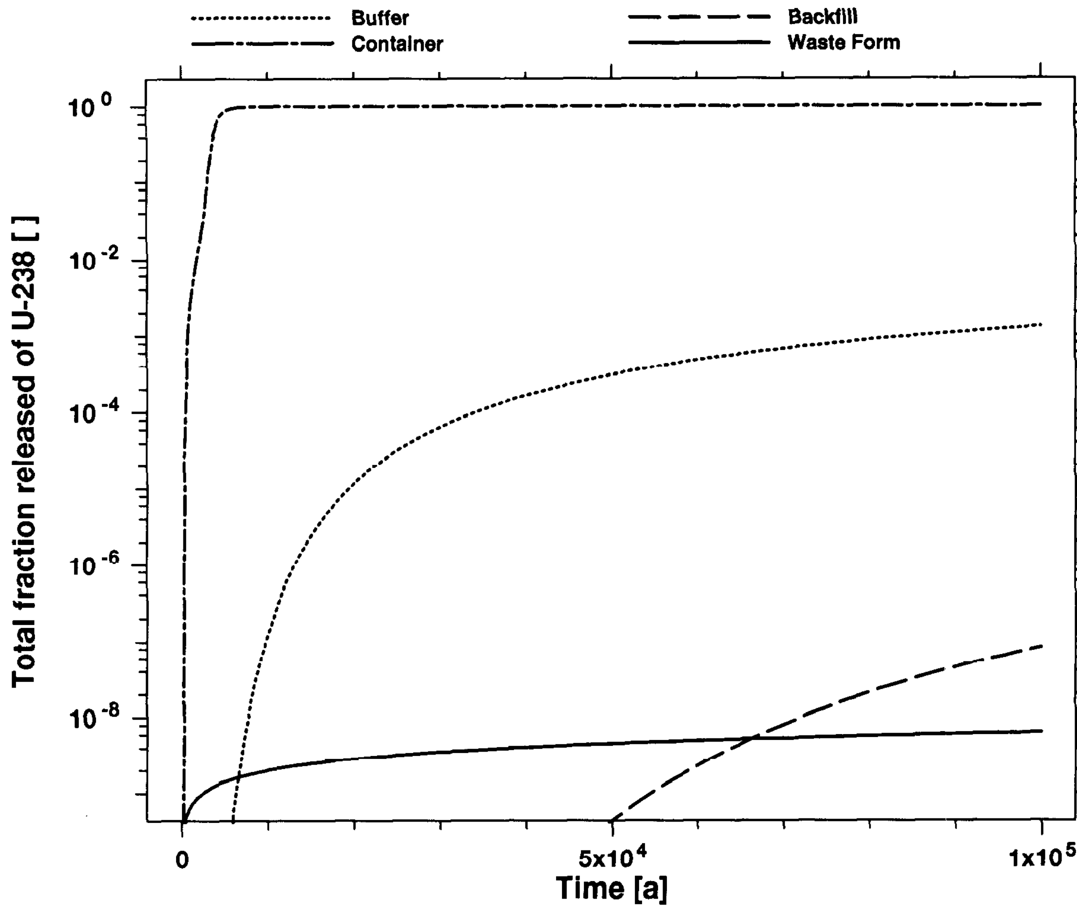

FIGURE D-66: Barrier Performance Measures for ^{238}U from Used Fuel

These four curves are calculated from the models for the four barriers: waste matrix, container, buffer and backfill. Not shown here are the curves for the rock within the geosphere because the total fractions released are less than 10^{-20} for times up to 10^5 a. The curves show the fraction released from each barrier as a function of time; this assumes a known amount of ^{238}U is instantaneously input to the barrier at time equal to zero. The vertical axis plots the total fraction released from the barrier (or the performance measure of the barrier for ^{238}U).
The most effective barrier for ^{238}U is the rock within the waste exclusion distance (not shown). Note that, because there are no instant releases of ^{238}U, the waste matrix is much more effective for ^{238}U than for ^{14}C, ^{129}I or ^{99}Tc.

- Fracture zone LD1, the containers and the buffer are less effective barriers, except at early times. The buffer does not significantly delay or attenuate releases of ^{14}C.

Iodine-129 displays a pattern similar to that for ^{14}C, except that the effects of radioactive decay are less significant (Figure 6-12 in the main text).

The pattern for ^{99}Tc is quite different. For this nuclide, precipitation is also an effective barrier because technetium is relatively insoluble. Figure D-65 shows that

- Precipitation limits the total fraction released to less than 10^{-2} for times up to 10^5 a. (The curve for the precipitation barrier shows a local maximum near 1000 a, which is attributed to variations in the rates of arrival of ^{99}Tc at its precipitate, and these variations are in turn attributed to variations in the number of containers failing at different times.)

- For ^{99}Tc, the backfill is the most effective barrier by many orders of magnitude, limiting the total fraction released to less than 10^{-7}. The buffer is also an effective barrier but with a larger limit of about 10^{-3}. Technetium-99 is strongly sorbed by both the buffer and backfill (Section D.2). However, the backfill is more effective because the volume of backfill is much greater than the volume of buffer.

- The rock within the 50-m waste exclusion distance is also very effective, more so than for ^{14}C and ^{129}I.

- The effectiveness of the backfill, buffer and rock within the waste exclusion distance are largely attributable to the sorption of ^{99}Tc on these media. Sorption of ^{99}Tc also occurs in fracture zone LD1, so that LD1-a and LD1-b are more effective barriers for ^{99}Tc than for ^{14}C and ^{129}I.

- The maximum fraction released from the waste matrix (used fuel) is less than 10^{-1} and is virtually entirely due to the initial inventory of ^{99}Tc available for instant release (with small losses due to radioactive decay). The instant-release inventory of ^{99}Tc is 6% in the median-value simulation (Section D.2).

Figure D-66 summarizes the effectiveness of different barriers for ^{238}U:

- The rock within the waste exclusion distance is extremely effective; it limits the total fraction released of ^{238}U to less than 10^{-20} for times up to 10^5 a, primarily because of sorption. The curve for this barrier is not shown in the figure because it plots below the minimum value shown.

- Sorption is also responsible for the effectiveness of the backfill, buffer and (not shown in the figure) the LD1 barriers.

- The waste matrix (used fuel) is also a very effective barrier, much more effective for ^{238}U than for ^{14}C, ^{129}I or ^{99}Tc. Comparison of Figures D-64 to D-66 and 3-12 shows that the total fraction released is more than 6 orders of magnitude smaller for ^{238}U. The waste matrix is an effective barrier for ^{238}U because this radionuclide is released only by the congruent-release mechanism, which depends on the solubility of the used-fuel matrix. Because the solubility of the used-fuel matrix solubility is small in the median-value simulation (1.55×10^{-7} mol/m^3), it follows that the total fraction of U-238 released is small. The waste matrix would also be an effective barrier for all other congruently released contaminants associated with used fuel and for all contaminants associated with the Zircaloy waste matrix (compare with Table 6-5 and Figures 6-13 and 6-14 in the main text).

D.9.2 CONSTRUCTION OF FIGURES 6-13 AND 6-14 IN THE MAIN TEXT

Figures 6-13 and 6-14 in Section 6.4 in the main text summarize the performance of the barriers for most of the radionuclides and the nine chemically toxic elements considered in the postclosure assessment. The first figure shows results at 10^4 a and the second, at 10^5 a. Two types of contaminants are not shown:

- The first type are radionuclides that are modelled using the secular-equilibrium approximation, including members of short decay chains (such as ^{93m}Nb from the radioactive decay of ^{93}Mo and ^{93}Zr) and some members of the actinide decay chains (such as ^{233}Pa from ^{237}Np). Section 5.9 in the main text lists all such radionuclides. They are not included in the analysis of barrier effectiveness because their effects are simulated only in the biosphere model, which does include any of the barriers evaluated here.

- The second type are radionuclides that are members of decay chains and whose inventory at any time is mostly due to ingrowth. In general, these radionuclides would exhibit the same behaviour as their precursors; for example, ^{236}U would behave much like ^{240}Pu. These radionuclides are identified in Figure 5-22 of Section 5.9 in the main text, with inventory data in Table 5-4.

We constructed Figures 6-13 and 6-14 (in Section 6.4 in the main text) as follows:

1. We first transform the data so that the results can be presented in a more informative fashion. We do this by calculating a "performance indicator" for each barrier and for each selected contaminant. It is proportional to the negative of the logarithm of the total fraction released (or performance measure). Values are calculated at 10^4 a for Figure 6-13 (main text) and at 10^5 a for Figure 6-14 (main text). For cases where the total fraction released is less than 9×10^{-38}, we assume a value of (about) 37 for the negative of the logarithm.

   With this data transformation, the barrier performance indicator ranges from zero (an ineffective barrier) to 37 (an extremely effective barrier). The smallest barrier performance indicator, zero, corresponds to a total fraction released (or performance measure) of unity, meaning that all of the contaminant has been released by the barrier. The largest value, 37, corresponds to a total fraction released of 9×10^{-38} or less, meaning that essentially none of the contaminant has been released.

2. These indicators are then used to illustrate the performance of the barriers for each contaminant. In the figures, the lengths of the boxes in the last eight columns are proportional to the barrier performance indicator. That is, longer boxes indicate

greater effectiveness of the barriers in attenuating and delaying contaminant releases.

3. We also calculate a "net performance indicator" by summing the barrier performance indicators for each contaminant. It is also equal to the negative of the logarithm of the net fractional release (Section 6.4 in the main text). When divided by the number of barriers, it is also equal to the average of the eight barrier effectiveness indicators or to the geometric mean of the eight total fractional releases.

   The net performance indicator for a contaminant is a pessimistic representation of the effectiveness of a sequential combination of the eight independent barriers in delaying and attenuating the release of the contaminant. Net performance indicators, shown in the first column of boxes in Figures 6-13 and 6-14 in the main text, are used to rank the list of contaminants. The length of a box is proportional to the net performance indicators. Thus contaminants near the bottom of the list, with longer boxes, are more attenuated and delayed than contaminants near the top of the list.

   In showing the boxes for net performance indicators, we actually plot the values of the net performance indicator divided by the number of barriers, which permits comparisons between net performance indicators and performance indicators for each barrier. The lengths of the boxes for the net performance indicators are equal to the average of the lengths of the boxes for the eight barrier performance indicators.

The results in Figures 6-13 and 6-14 in the main text are used to compare the performance of different barriers for different contaminants (Section 6.4 in the main text). In comparing different box lengths, it should be noted that the lengths are calculated using a negative logarithmic transform. Thus if barrier A has a box length <u>twice</u> that of barrier B, then the fractional release from barrier A is equal to the <u>square</u> of the fractional release from barrier B.

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APPENDIX E

DETAILED ANALYSES OF THE PROBABILISTIC SIMULATIONS

CONTENTS

continued...

CONTENTS (concluded)

E.1 INTRODUCTION

This appendix presents more details on selected topics related to the probabilistic analysis, or the analysis based on random sampling of parameter values from their probability density functions (PDFs). Appendix D discusses similar details on the analysis of the median-value simulation.

Section E.2 evaluates the implications of recent changes to the recommendations of the International Commission on Radiological Protection (ICRP). These changes affect both the estimation of annual dose estimates (ADEs) and the calculation of radiological risk, but they do not affect the overall conclusions of the assessment of the reference disposal system.

Section E.3 outlines the method for sensitivity analysis and identifies parameters that have a strong influence on the results. Sections E.4 to E.6 then discuss how these parameters affect the results from the vault, geosphere and biosphere models.

Section E.7 describes a special study of the tortuosity of the lower rock zone, the parameter that most affects the estimates of ADEs (Section 6.5.5 in the main text). The study shows how changes to the PDFs for tortuosity would affect estimates of annual dose.

Section E.8 presents details from another special study of the effects of selected site and design features.

E.2 IMPLICATIONS OF ICRP PUBLICATION 60

Canadian radiological requirements in Atomic Energy Control Board (AECB) Regulatory Document R-104 (AECB 1987) are based on the 1977 recommendations of the ICRP (ICRP 1977). In 1990, the ICRP revised its recommendations (ICRP 1991a); corresponding changes may be anticipated in Canadian requirements. The changes in the ICRP recommendations would affect estimates of radiation dose and radiological risk in this assessment in several ways. The two most important changes are

- The dose conversion factors (DCFs) used to calculate annual dose caused by radiation from different radionuclides would change. Values used in this report (and documented by Davis et al. 1993) are based on information in ICRP Publications 26 (1977), 30 (1979) and 56 (1989). Their values will eventually be replaced using new information from ICRP Publications 60 and 61 (ICRP 1991a,b). The new DCFs would increase for some radionuclides and decrease for others, typically by a factor of less than two.

  Of most importance to the postclosure assessment is the internal DCF for ^{129}I; it would increase from 9.7×10^{-9} to 1.6×10^{-8} Sv/Bq (Zach and Sheppard 1992), which would increase ADEs from ingestion of ^{129}I by about 60%. More details on these changes are provided in the primary reference for the biosphere model (Davis et al. 1993) and in a supporting document by Zach and Sheppard (1992) describing the food-chain model.

- Publication 26 (ICRP 1977) recommends the use of a conversion factor equal to 2×10^{-2} to calculate the associated risk of fatal cancers and serious genetic defects to an individual. Publication 60 (ICRP 1991a) recommends use of a nominal probability coefficient equal to 7.3×10^{-2} to calculate the risk of fatal and nonfatal cancers or severe hereditary effects. The revised recommendations imply a fourfold larger risk associated with a given exposure to radiation. Note that the details of the risk end points are not identical.

The results reported in Sections 6.3 and 6.5 in the main text can be recast as follows to allow for the above changes to the ICRP recommendations:

- For the median case deterministic simulation (Section 6.3 in the main text), ADEs from all radionuclides at 10^4 a would increase to about 5×10^{-18} Sv/a from 3×10^{-18} Sv/a; at 10^5 a, it would increase to about 6×10^{-7} Sv/a from 4×10^{-7} Sv/a.

- For the probabilistic results (Section 6.5 in the main text), ADEs from all radionuclides at 10^4 a would increase to about 1×10^{-11} Sv/a from 8×10^{-12} Sv/a; at 10^5 a it would increase to about 2×10^{-6} Sv/a from 1×10^{-6} Sv/a.

- The dose limit associated with the radiological risk criterion would be reduced if it were based on the new ICRP nominal probability coefficient. Using the AECB risk equation (AECB 1987) and an annual risk limit of 10^{-6} serious health effects per year, the corresponding associated dose limit would be 1.25×10^{-5} Sv/a. For both the deterministic and probabilistic calculations, the ADEs from all radionuclides, including the corrections noted above, would still be well below this dose limit.

In summary, we expect that the overall conclusions discussed in Section 6.5.2 and elsewhere in the main text would be unchanged following anticipated changes to regulatory requirements that reflect recent revisions to the ICRP recommendations. That is, the mean ADE to an individual in the critical group would still be much smaller than the dose limit associated with the radiological risk criterion over the entire simulation period of 10^5 a, and the corresponding risk of fatal and non-fatal cancers or severe hereditary effects would be far less than 10^{-6}/a.

E.3 SCREENING FOR IMPORTANT PARAMETERS

E.3.1 INTRODUCTION

Probabilistic sensitivity analysis examines the effects of changes to a parameter when all other parameters are free to vary across their entire ranges.

It is clear that changes in the value of an important parameter from one simulation to another can effect the magnitude of the maximum ADE that results from the simulations. Changing the distribution of an important parameter, either by changing its PDF or by using different sampling strategies, affects the probability of selecting particular values and, therefore, can affect the distribution of the maximum ADE. That is, changes to the distribution of an important parameter can change both the average value of the maximum ADE and the spread in its distribution.

In probabilistic sensitivity analysis, we first screen the thousands of sampled parameters to identify those that most influence some objective function, and then we investigate their effects. The screening method, iterated fractional factorial analysis, is similar to the one used for the deterministic sensitivity analysis (Sections 6.3.3 in the main text and D.5 in Appendix D), except that the selection of the parameter values is not restricted to values near the medians. Instead, the parameters are fixed in different simulations at the 0.01, 0.5 or 0.99 quantiles of their PDFs (values for the switch parameters are also varied to sample all important options). This choice permits examination of the effects of each parameter over its range of possible values, and allows direct comparison of the effects of parameters that have different physical units and different probability distributions.

Many different objective functions could be chosen for the analysis, such as time of maximum failure rate of the containers, rate of release of ^{129}I from the vault, rate of discharge of ^{14}C to the biosphere, ADEs at some point in time, estimated concentrations of radionuclides in the food chain, ADEs to nonhuman biota, and concentrations of chemically toxic elements in water, soil and air. As for the deterministic sensitivity analysis (Sections 6.3.3 in the main text and D.5 in Appendix D), we have focussed the probabilistic sensitivity analysis on the maximum ADE to individuals in the critical group, taken for times up to 10^5 a and resulting from the radionuclides ^{14}C and ^{129}I. We also consider the arithmetic average or mean value of the maximum ADE, summed over all radionuclides. These ADEs were chosen as the primary objective functions because

- Radiation doses to the critical group are deemed to be of most concern.

- The results in Section 6.5 in the main text show that doses from ^{14}C and ^{129}I dominate the ADEs up to 10^5 a.

- We are most interested in parameters that are important in the estimate of risk, because the radiological risk criterion (AECB 1987) is used to examine the overall performance of a disposal system. The radiological risk estimate for a scenario is proportional to the arithmetic average of the ADE (AECB 1987). However, our results (for the SYVAC scenarios) indicate that the arithmetic average is dominated by a few simulations that have large ADEs (Sections 6.5.1 and 6.5.2 in the main text) and, therefore, it is reasonable to examine the maximum ADEs. We consider the maxima up to 10^5 a, the entire period for which the models can provide reasonably reliable quantitative results.

- The statistics using maxima to 10^5 a are more reliable than maxima to 10^4 a because they are based on more nonzero data points. It is readily shown, for instance, that the statistical convergence is superior for the mean of the maximum ADE up to 10^5 a than for the mean of the ADE at any specific time between zero and 10^5 a. More useful statements can be made for data that have better convergence.

- It is conservative to choose the longer period, in the sense that maximum ADEs observed for times up to 10^5 a are larger (and cannot be smaller) than maximum ADEs up to 10^4 a.

- Likewise the mean of the maximum ADEs observed for times up to 10^5 a are larger than the mean of the maximum ADEs up to 10^4 a. Moreover, the mean of the maximum ADEs is an upper bound on the maximum of the mean ADEs. In general, the radiation doses from the disposal system would not be underestimated when using the mean of the maximum ADE.

One other practical consideration favours the use of the maximum ADE from individual simulations as the objective function. With this choice, we can apply the fractional factorial screening method (Section A.4, Appendix A). It is not feasible to use this method with the mean ADE as the objective function because the method can be readily applied only to individual simulations from a set of selected simulations, and not to summary results from a set of randomly sampled simulations.

We recognize that different objective functions will yield different results. For example, if the function of interest is the ADE at 250 a, then screening studies would almost certainly identify parameters related to corrosion of the containers. Nevertheless, we believe that a more appropriate objective function is the maximum of the estimated radiation dose, taken over as long a time frame as is feasible. The screening studies using such functions will then tend to identify parameters that affect attenuation of impacts, rather than parameters that merely delay impacts.

As used in this document, therefore, an important parameter is one that has a notable effect on the maximum ADE or the mean of the maximum ADE, when considering the full range of uncertainty of the important parameter and the full range of uncertainty of all other parameters.

Nevertheless, we have performed other screening studies to identify parameters that have important effects on results calculated by the vault, geosphere and biosphere models. For these ancillary screening studies, we use objective functions called performance measures:

- The vault performance measure for ^{129}I is defined as the total estimated amount (in moles) of ^{129}I released from the vault up to 10^5 a. A similar measure is defined for ^{14}C.

- The geosphere performance measure for ^{129}I is defined as the total amount of ^{129}I that leaves the geosphere divided by the total amount of ^{129}I that enters the geosphere, over 10^5 a. A similar performance measure is defined for ^{14}C.

- The biosphere performance measure for ^{129}I is defined as a ratio of integrals for times up to 10^5 a: an interim integral of the ADE from ^{129}I is divided by the total amount of ^{129}I that enters the biosphere. The biosphere performance measure has units of Sv/mol, and it provides an approximation of the total radiation dose from the arrival of one mole of ^{129}I at the biosphere. A similar performance measure is defined for ^{14}C.

  For both radionuclides, the "interim" integral excludes the effects of isotopic dilution (Section 5.6 in the main text), which tends to obscure some effects.

These performance measures isolate particular components of the system model and help to identify additional influential parameters. We include an evaluation of how these additional parameters affect the ADEs.

In the following sections, we summarize the results of the screening analysis (Section E.3.2), and then describe three studies aimed at confirming that all important parameters have been identified (Section E.3.3). Sections E.4 to E.6 discuss how the identified parameters affect the ADEs and the vault, geosphere and biosphere performance measures.

E.3.2 IDENTIFICATION OF IMPORTANT PARAMETERS

Section 6.5.5.3 and Table 6-13 in the main text list eight parameters found to be most important for the reference disposal system: they have the largest influences on the maximum ADE up to 10^5 a. These eight parameters are referred to as the "important" parameters.

Table E-1 lists another 18 parameters known as the "less important" parameters. They were selected primarily because they have notable effects on the performance measures for the vault, geosphere or biosphere models. (A few were also selected because expert opinion suggested they might be important in some conditions.) They are "less" important in the sense that their effects on the maximum ADE are much weaker than the eight important parameters in Table 6-13 (Section 6.5.5.2 in the main text).

Correlation coefficients are calculated from 500 randomly sampled simulations, using logarithms of the variable (performance measure or maximum ADEs) and parameter value. Correlation coefficients vary between +1 and -1; a value of +1 (-1) means that the logarithm of the variable is linearly dependent on the logarithm of the parameter, and it increases (decreases) as the parameter value increases. A correlation coefficient equal to zero implies that there is no linear relationship between the variable and the parameter. For example, results in Table E-1 for "aquatic mass loading coefficient for iodine" show that a definite relationship exists, whereas "initial system potential" has essentially no effect.

TABLE E-1

LESS IMPORTANT PARAMETERS FOR THE PROBABILISTIC SIMULATIONS

Parameter	Model and Nuclide*	Correlation Coefficient** for Model Performance	Maximum ADE
Aquatic mass loading coefficient for iodine	B,I	0.26	0.22
Gaseous evasion rate from soil for iodine	B,I	-0.25	-0.16
Initial inventory of ^{129}I	V,I	0.53	0.13
Plant/soil concentration ratio for iodine	B,I	0.20	0.10
Backfill anion correlation parameter	V,I	-0.15	-0.07
Instant-release fraction of ^{129}I	V,I	0.14	0.08
^{129}I plant environmental half-life	B,I	0.05	0.05
Switch selecting use of lake sediment as soil***	B,C	0.10	0.05
Initial inventory of ^{14}C	V,C	0.74	-0.04
Plant/soil concentration ratio for carbon	B,C	0.13	0.03
Gaseous evasion rate from soil for carbon	B,C	-0.15	-0.03
Size of the critical group	G,C	0.06	-0.03
Retardation factor of carbon in compacted organic lake sediment	B,C	-0.20	-0.02
Thickness of overburden at Boggy Creek South	G,C	-0.09	-0.02
Free-water diffusion coefficient for carbon	G,C	0.18	-0.01
Plant to mammalian meat coefficient for carbon	B,C	0.03	0.01
Instant-release fraction of ^{14}C	V,C	0.42	-0.01
Initial System Potential	V,I	0.03	0.00

* Model and nuclide indicate which performance indicator is cited in the column. The abbreviations used are V, G and B for vault, geosphere and biosphere respectively, and I and C for ^{129}I and ^{14}C respectively.

** For "Maximum ADE," the data are the maximum ADEs from ^{14}C and ^{129}I and the parameter values. Data are from a set of 500 randomly sampled simulations.

*** For this switch parameter, biosphere performance measures and ADEs are generally greater when the sediment is used as soil.

We also refer to the remaining parameters, about 1300 in all, as the "unimportant" parameters. (SYVAC3-CC3 uses about 1400 sampled parameters in simulations involving ten nuclides (Section A.3.3, Appendix A). Our analysis is concentrated on the seven radionuclides (^{14}C, ^{135}Cs, ^{129}I, ^{59}Ni, ^{107}Pd, ^{79}Se and ^{99}Tc from used fuel) that were initially expected to be major contributors to the ADE. The subsequent set of sampled parameters numbers just over 1300.)

The relative influence of the important, less important and unimportant parameters is discussed in Section 6.5.5.2 in the main text, based on a calculation of coefficients of determination (Section A.4 in Appendix A) for sets of 500 simulations in which different combinations of the three classes of parameters were randomly sampled. The results (Table 6-14 in the main text) show that most of the variability in the estimates of maximum annual dose is explained by the uncertainty in the eight important parameters. A small fraction can be explained by the 18 less important parameters, and very little is attributed to the 1300 unimportant parameters.

These observations provide strong evidence that Table 6-14 in the main text contains all the important parameters. We provide further confirming studies in the following section.

The analysis of effects in Sections E.4 to E.6 concentrates on the more important parameters:

- the eight important parameters listed in Table 6-13 in the main text that have the largest effects on the ADE; and

- those of the 18 less important parameters in Table E-1 that have the largest effects on the performance measures for the vault, geosphere and biosphere.

E.3.3 CONFIRMING STUDIES

Three supporting studies were aimed specifically at confirming the completeness of Table 6-13 in the main text: pairwise comparisons, regression analysis and extreme-simulation analysis.

E.3.3.1 Pairwise Comparisons

Pairwise comparisons use sets of randomly sampled simulations, involving special sampling strategies for different classes of parameters. In this case, we examine three classes: the eight important parameters (Table 6-13), the 18 less important parameters (Table E-1) and the remaining sampled parameters, totalling approximately 1300.

Five sets of 500 simulations are used in the pairwise comparisons. In four of the sets, the sampling of the parameter values was altered to isolate the cumulative effects of important, less important and unimportant parameters. A description of these sets follows.

- In Set 1, all parameters are randomly sampled from their PDFs. This is the reference set; in fact, it is the first 500 random simulations used in the probabilistic analysis (Section 6.5 in the main text).

- In Set 2, all unimportant parameters use the same sequence of 500 randomly selected values as in Set 1. The 18 less important and eight important parameters are fixed at their median values in all 500 simulations.

- In Set 3, all unimportant parameters are fixed at their median values. The eight important and 18 less important parameters have the same sequence of 500 randomly selected values as in Set 1.

- In Set 4, all unimportant and less important parameters use the same sequence of 500 randomly selected values as in Set 1. The eight important parameters are fixed at their median values in all 500 simulations.

- In Set 5, all unimportant and less important parameters are fixed at their median values. The eight important parameters have the same sequence of 500 randomly selected values as in Set 1.

Figure E-1 illustrates the results and shows that

- In part (a) of the figure, the maximum ADEs from each of 500 simulations in Set 1 are plotted against the corresponding estimates from Set 2. The maximum ADEs from Set 1 range over 9 orders of magnitude, whereas the equivalent results from Set 2 vary over only 2 orders of magnitude. That is, there is a large reduction in the variability of the maximum ADEs when the important parameters are fixed at their median value. This indicates that important parameters have a large effect on the variability in the maximum ADE.

- Part (b) of the figure plots the maximum ADEs from the 500 simulations in Set 1 against the corresponding estimates from Set 3. In this case, there is little difference in variability in the two sets of doses, confirming that the unimportant parameters have little effect on the variability in the maximum ADEs.

- Parts (c) and (d) of the figure plots the maximum ADEs in Set 1 against the corresponding estimates in Sets 3 and 4. We observe that the range of variation along the vertical axis is somewhat larger in part (c) compared with part (a) and in part (d) compared with part (b). These results confirm that the 18 less important parameters also affect the variability in the maximum ADEs, and that they are, indeed, less important.

We also present in Table E-2 the arithmetic averages and confidence limits of the maximum ADEs to 10^5 a for each of the five sets of results, along with results from the median value simulation (Section 6.3 in the main text), in which all parameters are fixed at their median values. The results show that

- Comparison of Sets 1, 3, and 5, and the median-value simulation, show a trend in the mean of the maximum estimated dose. The means are almost the same for Sets 1 and 3: 1.2×10^{-6} and 1.0×10^{-6} Sv/a. However, there is a large decrease when the 18 less important parameters are fixed and another decrease when all parameters are fixed (the median-value simulation).

- The median-value simulation and Sets 2, 4, and 1 show a related trend: the means of the maximum estimated dose are smallest for the median-value simulation, slightly larger when the 1300 unimportant parameters are sampled (Set 2), larger still when the 1300 unimportant and 18 less important parameters are sampled (Set 4), and largest when all parameters are sampled (Set 1).

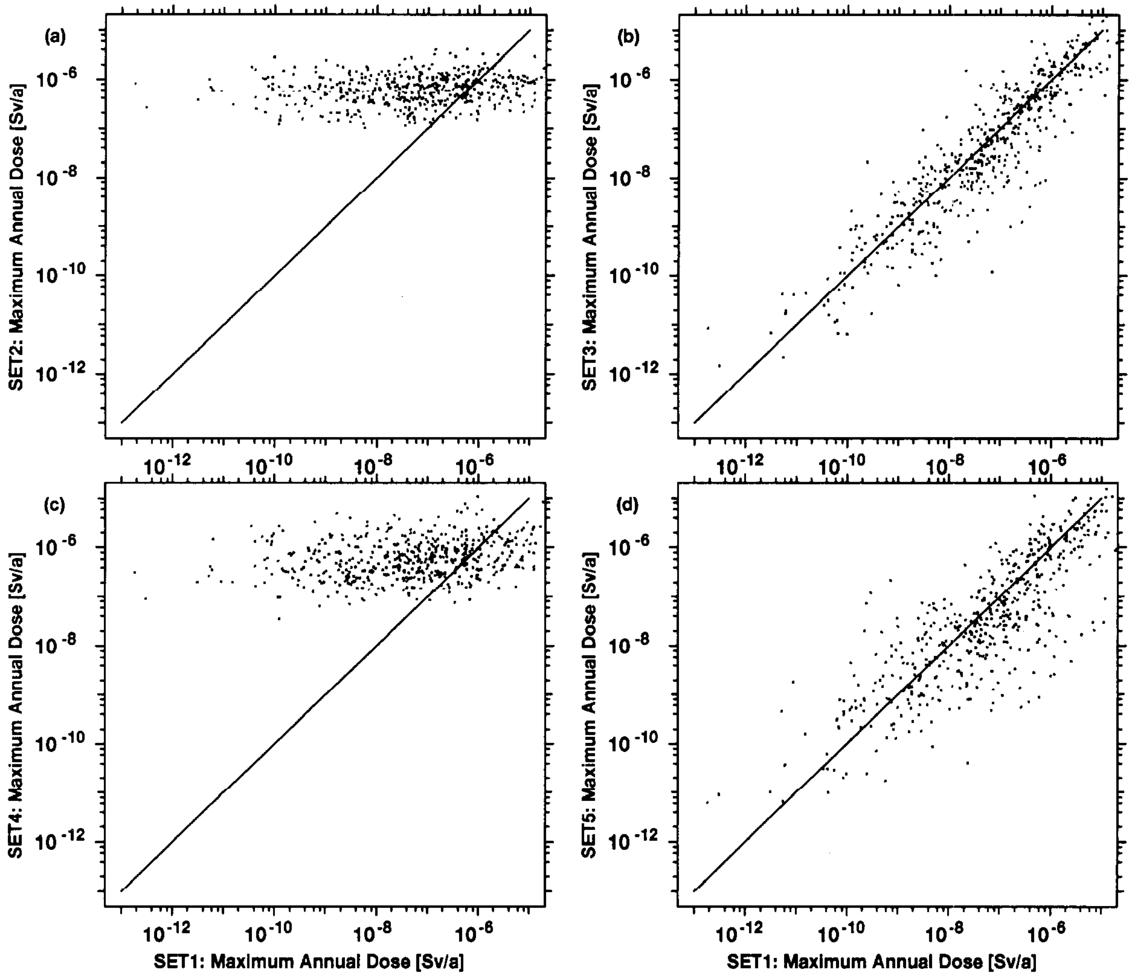


FIGURE E-1: Pairwise Comparisons Involving the Important Parameters

These scatter plots compare maximum estimated annual doses for times up to 10^5 a from five sets of 500 randomly sampled simulations. Each point locates a pair of related simulations: the horizontal axis locates the result from a simulation belonging to Set 1, and the vertical axis locates the result from the corresponding simulation belonging to Set 2 (or Sets 3 to 5). The parameter values used in a simulation for Sets 2 to 5 are identical to the parameter values used in the related simulation for set 1, except that the following parameters are fixed at their median values for all 500 simulations (Table E-2):

- In Set 2—the eight important and 18 less important parameters;
- In Set 3—the unimportant parameters;
- In Set 4—the eight important parameters; and
- In Set 5—the unimportant and less important parameters.

Pairwise comparisons of these sets reveal the effects of the important, less important and unimportant parameters:

- Part (a) shows the results from Set 1 (horizontal axis) plotted against those from Set 2 (vertical axis). The results would fall on the diagonal line if they were identical; the pairwise comparison shows that the variability of maximum estimated annual doses in Set 2 is much smaller than the variability in Set 1.
- Part (b) shows the results from Set 1 (horizontal axis) compared with Set 3 (vertical axis); there is much less difference between these pairs of simulations.
- Parts (c) and (d) show Set 1 (horizontal axis) compared with Sets 4 and 5 (vertical axes) and confirm that the 18 less important parameters are less important.

TABLE E-2

SUMMARY OF THE PAIRWISE COMPARISONS*

Simulation Set	Parameter Values: 8 Important Parameters	18 Less Important Parameters	1300 Unimportant Parameters	Annual Dose: Mean of Max. Dose (Sv/a)	95% Conf. Limit* (Sv/a)	Coefficient of Determination (R^2)** to 10^4 a	10^5 a
1	random	random	random	1.2×10^{-6}	4.4×10^{-7}	1.00	1.00
3	random***	random***	median	1.0×10^{-6}	3.6×10^{-7}	0.86	0.83
5	random***	median	median	6.3×10^{-7}	1.9×10^{-7}	0.84	0.67
m	median	median	median	4.0×10^{-7}	-	-	-
2	median	median	random***	7.8×10^{-7}	7.3×10^{-8}	0.04	0.03
4	median	random***	random***	9.4×10^{-7}	1.1×10^{-7}	0.04	0.07

* These comparisons are used to show the effects of three categories of parameters: the eight important parameters (Table 6-13 in the main text), the 18 less important parameters (Table E-1), and approximately 1300 other unimportant parameters. The columns labelled "parameter values" give the characteristics of five sets of 500 simulations; the label "m" corresponds to the (single) median-value simulation discussed in Section 6.3. The last three columns give results for each set:

- "Mean of Max Dose" is the arithmetic average of the maximum ADEs for times up to 10^5 a;
- "95% Confidence Limit is an associated confidence limit (Section A.3.5, Appendix A); and
- The coefficients of determination are from a linear regression (Section A.4) on the logarithms of the maximum ADEs for times up to 10^4 or 10^5 a.

** Coefficients of determination (or R^2) are calculated using logarithms of the maximum ADEs to 10^5 a from the seven radionuclides contributing most to the maximum ADEs (notably ^{14}C and ^{129}I). The calculations use the maximum ADEs from simulation Set 1 and the maximum ADEs from each of the other indicated simulation sets.

*** These parameters use the identical sequence of randomly selected values as is used in set 1.

- The results also show a trend of decreasing values of the confidence limit from Sets 1 to 3 to 5 and from Sets 1 to 4 to 2.

These trends indicate that the eight important parameters affect both the magnitude of the mean maximum ADE and its associated variability. Figure 6-20 in the main text clearly illustrates these effects in plots of annual dose versus time for sets 1, 4 and 5.

The last column in Table E-2 is also revealing; it suggests that (as expected) Set 3 is most similar to Set 1, followed by Set 5. Sets 2 and 4 are significantly different from Set 1.

In summary, the pairwise comparisons provide strong evidence that Table 6-13 in the main text has identified the most important parameters affecting the maximum ADEs.

E.3.3.2 Regression Analysis

A second study compares results from regression analysis with similar results obtained using iterative fractional factorial analysis. As indicated below, both analyses identify the same parameters as most important. To simplify the regression analysis, we restrict the study to the vault model and make some simplifying assumptions noted below. One restriction is that both analyses are aimed at identifying the important parameters that affect the total estimated releases of ^{14}C and ^{129}I from the vault for times up to 10^5 a.

Linear regression analysis is commonly used to measure the linearity of the relationships between parameters in a system (Section A.4, Appendix A). In this study, we can make use of the fact that the characteristics of the equations of the system are known. We use this knowledge to enhance linear regression analysis to measure nonlinear relationships between parameters in the system.

For the vault model, most of the parameters appear as multiplicative factors or as part of terms that are multiplicative. When we take the logarithm of a multiplicative relation, a linear relation is obtained. Therefore, we assume in the regression analysis that the responses of interest (the total estimated releases of ^{14}C and ^{129}I) are each a product, denoted by Y, of the input variables of interest, denoted by X_i in the expression

$$Y = b_0 \cdot X_1^{b_1} \cdot X_2^{b_2} \cdot X_3^{b_3} \; . \; . \; . \; ,$$

where the variable, X_1, is raised to the power b_1, X_2 is raised to power b_2, and so forth. The logarithmic version of this expression is

$$\log(Y) = \log(b_0) + b_1 \log(X_1) + b_2 \log(X_2) + \; . \; . \; . \; .$$

Because the unknown factors, b_i, now appear as multipliers in a linear equation, they can be estimated by minimizing the sum of the squares of the deviations of the calculated values of $\log(X_i)$ from the best straight line fitted to all the data.

We can use this approach to estimate the contribution to the variation of log(Y) from each of the $\log(X_i)$. The formula used to estimate these contributions is given in Section A.4, Appendix A; it results in a value for the coefficient of determination, R^2. An R^2 value provides an estimate of the portion of the variability in the response that is due to the range of possible values of the parameter. Values of R^2 range from 0 to 1: a value of 0 means that none of the variability in the response is associated with the selected parameter, and a value of 1 means that all the variability of the response is attributed to the parameter.

For efficiency of computation, we employed expert judgment to exclude from the regression analysis most of the parameters used in the vault model.

For instance, all constant parameters, and those pertaining to nuclides other than ^{14}C and ^{129}I were excluded. We also excluded all parameters used in the calculations of solubilities of radionuclides, because neither ^{14}C nor ^{129}I precipitate in the buffer in any simulation. Table E-3 lists the 15 remaining parameters; six are nuclide specific, whereas the remaining nine apply to all nuclides (thus 12 parameters affect ^{129}I releases, and 12 affect ^{14}C releases).

For the iterated fractional factorial analysis, no parameters were excluded. Thus the iterated fractional factorial analysis considered more than 1300 parameters, whereas the regression analysis considered just 15 parameters.

Two variations on regression analysis were applied to total releases of ^{14}C and ^{129}I from the vault up to 10^5 a.

- An R^2 value was calculated for the logarithm of the ^{129}I release and the logarithm of five parameters: the initial inventory of ^{129}I, the instant-release fraction of ^{129}I, the buffer anion correlation parameter, the groundwater velocity scaling factor, and the tortuosity of the lower rock zone. An R^2 value of 0.92 was obtained, indicating that the variation of these five parameters accounts for about 92% of the variation of the logarithm of the ^{129}I release. In other words, the variability in the logarithm of estimated releases of ^{129}I is nearly all due to the combined uncertainty of the five parameters. Similarly, an R^2 value was calculated for the logarithm of the ^{14}C release and the logarithm of five parameters: the initial inventory of ^{14}C, the instant-release fraction of ^{14}C, the buffer anion correlation parameter, the groundwater velocity scaling factor and the tortuosity of the lower rock zone. The resulting R^2 value of 0.88 indicates that these five selected parameters collectively account for a large portion of the variability in the total release of ^{14}C to 10^5 a.

- To quantify the importance of a single parameter, R^2 values were calculated for the logarithm of vault release and the logarithm of individual parameters. The results are given in Table E-3. We use the values of R^2 for the logarithm of the parameter in the regression analysis. The table also shows, for comparison, a ratio of results from the iterated fractional factorial analysis.

As indicated in the table, these results show good consistency with the results from the fractional factorial analysis. Both methods clearly identify the first four important parameters for ^{14}C: its initial inventory, its instant-release fraction, the buffer anion correlation parameter, and the groundwater velocity scaling factor. Both also clearly identify the first four important parameters for ^{129}I: its initial inventory, the buffer anion correlation parameter, the groundwater velocity scaling factor, and the tortuosity of the lower rock zone.

We conclude from this comparison that fractional factorial analysis is capable of identifying the important parameters in a complex model subject to considerable variability, adding to our confidence in the results presented in Tables 6-13 (in the main text) and E-2.

TABLE E-3

COMPARISON OF RESULTS FROM REGRESSION ANALYSIS AND FRACTIONAL FACTORIAL ANALYSIS*

Parameter	R^2 Value for Estimated Release of ^{14}C	R^2 Value for Estimated Release of ^{129}I	Relative Importance for ^{14}C	Relative Importance for ^{129}I
Initial inventory of ^{14}C	0.55	**	100	**
Initial inventory of ^{129}I	**	0.28	**	9.9
Instant-release fraction of ^{14}C	0.17	**	19	**
Instant-release fraction of ^{129}I	**	0.02	**	1.6
Buffer anion correlation parameter	0.13	0.31	16	8.6
Groundwater velocity scaling factor	0.06	0.21	13	9.7
Tortuosity of the lower rock zone	0.01	0.08	-1.7	-2.2
Backfill anion correlation parameter	0.01	0.02	-1.3	-1.7
Free-water diffusion coefficient (carbon)	0.01	**	2.1	**
Free-water diffusion coefficient (iodine)	**	0.01	**	-
Dispersivity, lower rock zone	<0.01	<0.01	3.0	1.1
Mean corrosion rate, cool containers	0.01	<0.01	1.8	1.2
Mean corrosion rate, cold containers	<0.01	<0.01	-1.5	-1.5
Mean corrosion rate, hot temperatures (short times)	<0.01	<0.01	2.4	1.5
Mean corrosion rate, hot temperatures (long times)	0.01	0.01	3.1	1.4

* These results are from two analyses that examine the variability in the total estimated releases from the vault of ^{14}C and ^{129}I to 10^5 a. The regression analysis examines the effects of the ranges of values for only 15 parameters, whereas the fractional factorial analysis includes the effects of more than 1300 parameters (results are shown only for the 15 of interest). Both analyses use logarithmic transformations of the data.
The first two columns of data are coefficients of determination or R^2 (Appendix A, Section A.4) from the regression analysis. Based on studies of similar data, we would expect that these values of R^2 are accurate to within about ±0.04 units. Dashes (-) indicate that the R^2 value is close to zero or the relative importance is close to unity and, therefore, that the indicated parameter has little effect.
The "Relative Importance" data are ratios of the geometric means of estimated releases from the vault from 512 simulations using fractional factorial analysis: the geometric mean from simulations using 0.99 quantile values is divided by the geometric mean of simulations using 0.01 quantile values. If this ratio is less than unity, its reciprocal is taken to permit more ready comparison of the relative importance of different parameters. A positive ratio indicates that the estimates tend to increase as the parameter values increase. A negative sign indicates the reverse pattern (and that the original ratio was less than unity).

** The parameters are specific to another radionuclide and do not affect the estimated release or relative importance.

E.3.3.3 Extreme-Simulation Analysis

Another test of the results in Table 6-13 in the main text involves examination of large- and small-dose simulations. The large- and small-dose simulations are those yielding the largest and smallest estimates of maximum annual dose for times up to 10^5 a. From the first 9000 randomly sampled simulations, we selected for study the 20 simulations with the largest and the 20 simulations with the smallest estimates of maximum annual dose. We then examined the values used in these simulations for the eight important parameters.

The results for the most important parameter, the tortuosity of the lower rock zone, were consistent. Its values in the large-dose simulations were all small, generally less than the value corresponding to its 0.10 quantile, whereas its values in the small-dose simulations were all large, greater that its 0.90 quantile value. That is, large-dose simulations consistently tend to have small values of tortuosity, and small-dose simulations consistently tend to have large values of tortuosity. (However all simulations with small values of tortuosity are not necessarily large-dose simulations.) These trends conform with the deterministic sensitivity analysis describing the effects of the tortuosity of the lower rock zone (Section D.7, Appendix D).

Similar strong correlations were also observed for the switch controlling the source of domestic water; for example, the well was selected in 19 of the 20 large-dose simulations, conforming with the results of the deterministic sensitivity analysis.

The remaining six parameters in Table 6-13 in the main text showed similar trends but were not as consistent. These weaker correlations are expected because these parameters are much less important than the tortuosity of the lower rock zone.

E.4 SENSITIVITY ANALYSIS OF THE VAULT MODEL

E.4.1 IMPORTANT PARAMETERS OF THE VAULT MODEL

The screening of parameters from the probabilistic simulations of the system model has identified three important parameters used in the vault model (Table 6-13 in the main text). These parameters are important in the probabilistic simulations in the sense that variations from their 0.01 to 0.99 quantiles result in notable changes to the maximum ADEs. The three important parameters are

- Tortuosity of the lower rock zone (a measure of the increase in the effective distance for transport by diffusion resulting from the winding nature of the interconnected aqueous pathway);

- Groundwater velocity scaling factor (describes uncertainty in groundwater velocities in the transport network and is used in such a way that groundwater velocities in all segments are increased or decreased by the same fraction); and

- Buffer anion correlation parameter (correlates the values of the buffer diffusion coefficient and the buffer capacity factor for all contaminants in the vault that are expected to form anionic species in groundwater).

The first two parameters are normally associated with the geosphere model, but they affect the vault model through the linkages between the vault and geosphere models (Section 5.3 in the main text).

Another fractional factorial screening study and a linear correlation analysis were directed at the vault performance measures for ^{129}I and ^{14}C. The vault performance measure for ^{129}I is defined as the total estimated amount of ^{129}I released from the vault up to 10^5 a; a similar performance measure is defined for ^{14}C. From these studies, three additional parameters have a strong effect on the two vault performance measures (Tables E-1 and E-3):

- the initial inventory of ^{14}C in used fuel;

- the initial inventory of ^{129}I in used fuel; and

- the instant-release fraction for ^{14}C (the fraction of the ^{14}C inventory located in the gaps and grain boundaries of the fuel pellets, which we assume is released to the void spaces within the interior of the container at the time of container failure).

One other parameter

- the instant-release fraction for ^{129}I (the fraction of the ^{129}I inventory located in the gaps and grain boundaries of the fuel pellets, which we assume is released to the void spaces within the interior of the container at the time of container failure),

also appears (but has weak effects) in Table E-1. We consider it further in the discussion below to round out the discussion on the effects of initial inventories and instant-release fractions. Two other parameters in Table E-1, the backfill anion correlation parameter and the initial system potential, have weak effects and are not discussed further.

The seven parameters listed above are the same as those identified in the sensitivity analysis of the median-value simulation (Section 6.3.3 in the main text).

Scatter plots are used to show the effects of these seven important parameters on the vault performance measures for ^{129}I and ^{14}C and on the maximum ADE up to 10^5 a from ^{129}I and ^{14}C. Each plot is presented using logarithmic scales to display the large range of values for the estimated variables that were obtained from the first 10 000 simulations of the probabilistic analysis.

Each plot also includes a trend line and the associated 95% confidence bands. The trend line (or regression line) is the least-squares fit (Section A.4.3.2, Appendix A) to the logarithm of the parameter values and the logarithm of the estimated variables. The associated 95% confidence bands put bounds on the location of this trend line (Section A.4.3.3, Appendix A).

Correlation coefficients measure the extent to which the data fits the regression line (Section A.4.3.2, Appendix A). The degree of spread of data points about the trend line is a reflection of the effects of the ranges of possible values of the other parameters. Correlation coefficients vary between -1 and +1:

- A correlation coefficient of +1 means that the logarithm of the estimated result is linearly dependent on the logarithm of the parameter and increases as the parameter value increases. A coefficient of +1 would occur when all plotted values in the scatter plot fall on the trend line.

- Similar comments apply to a correlation coefficient of -1, except that the estimated result decreases as the parameter value increases.

- A correlation coefficient equal to zero implies that there is no linear relationship between the estimated variable and the parameter and that there is a wide spread of plotted points about the trend line.

Table E-4 shows the correlation coefficients calculated for the seven parameters from the figures discussed in Sections E.4.2 to E.4.4. The results in the table show that

- For most parameters, the correlation coefficients are closer to +1 or -1 for the vault performance measures than for the maximum ADE. This occurs because of the added uncertainty of parameters not used in the vault model that affect the ADEs.

- For two parameters, the reverse pattern occurs. The correlation coefficients pertaining to the tortuosity of the lower rock zone and the groundwater velocity scaling factor (for ^{14}C) are closer to ±1 for the maximum ADE. This reversal occurs because these two parameters are also used in the geosphere model, where they have strong effects on the ADE (Section E.5).

- The first three parameters in the list have large correlation coefficients for maximum ADE from ^{129}I; that is, these three parameters show the largest effects on the estimates of maximum annual doses from ^{129}I. This confirms the relative importance of these three parameters to maximum ADE from all radionuclides (Table 6-13 in the main text), because ^{129}I is the major contributor to dose for times up to 10^5 a.

Table E-4 also indicates the initial inventory of ^{129}I in used fuel and the groundwater velocity scaling factor are approximately equally significant to the maximum ADE to 10^5 a resulting from ^{129}I. This appears to contradict Table 6-13, which does not include the initial inventory of ^{129}I in used fuel as an important parameter. In fact, the results are not contradictory: the difference is attributable to the different methods of analysis. In Table 6-13 in the main text, the parameters are ranked according to the fractional factorial screening analysis, in which parameter values are either near the ends or in the centre of the range of possible values (at the 0.01, 0.99 or 0.50 quantiles). In Table E-4, parameter values are

TABLE E-4

CORRELATION COEFFICIENTS SUMMARIZING EFFECTS OF SEVEN IMPORTANT VAULT PARAMETERS*

Parameter	Correlation Coefficients: Releases from the vault for ^{14}C	^{129}I	Maximum Annual Dose from ^{14}C	^{129}I
Tortuosity of the lower rock zone	-0.12	-0.28	-0.45	-0.55
Groundwater velocity scaling factor	0.25	0.46	0.36	0.12
Buffer anion correlation parameter	0.36	0.56	0.10	0.18
Initial inventory of ^{14}C in used fuel	0.74	**	0.18	**
Initial inventory of ^{129}I in used fuel	**	0.53	**	0.13
Instant-release fraction for ^{14}C	0.42	**	0.12	**
Instant-release fraction for ^{129}I	**	0.14	**	0.08

* These correlation coefficients are calculated from the plots discussed in Sections E.4.2 to E.4.4; they reflect the spread of results about a trend line. A correlation coefficient equal to zero implies that there is no relationship between the estimated variable and the parameter and that there is a wide spread of plotted points about the trend line. Correlation coefficients of +1 or -1 imply that there is a linear relationship between these parameters.
These data were obtained from a set of 10 000 randomly sampled simulations. Confirmation studies, using four sets of 1000 randomly sampled simulations, produce similar results; for example, 90% of the results from all four sets agree to within ±0.04 units.

** The parameters are specific to another radionuclide.

selected randomly according to their assigned PDFs. This means that, with respect to the extremes of the PDFs, the initial inventory of ^{129}I is not a comparatively important parameter, but it is equally as important as the groundwater velocity scaling factor on the basis of random sampling.

E.4.2 EFFECTS OF INVENTORIES AND INSTANT-RELEASE FRACTIONS

Figures E-2 to E-5 are scatter plots showing the effects of the initial inventories of ^{14}C and ^{129}I and the instant-release fractions of ^{14}C and ^{129}I:

- Parts (a) of the figures show the effects on the vault performance measure for ^{14}C or ^{129}I, and

- Parts (b) show the effects on the maximum ADEs from ^{14}C or ^{129}I.

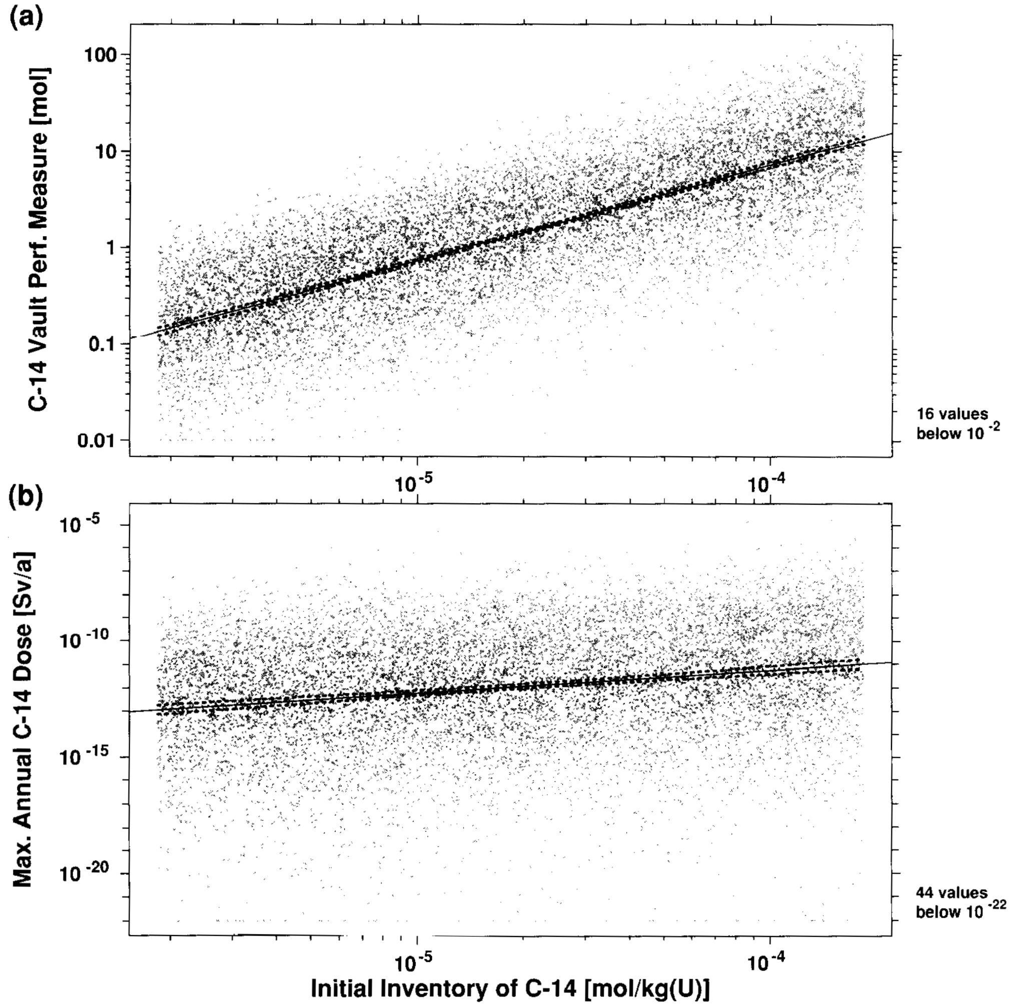


FIGURE E-2: Effect of the Initial Inventory of ^{14}C

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the initial inventory of ^{14}C in used fuel. The vertical axes are

(a) the vault performance measure for ^{14}C, defined as the total estimated amount of ^{14}C released from the vault up to 10^5 a; and

(b) the maximum annual dose estimate from ^{14}C up to 10^5 a.

The correlation coefficients for the trend lines are 0.74 for the vault performance measure, and only 0.18 for the maximum annual dose estimate, indicating that parameters for the geosphere and biosphere models contribute additional variability. The slopes of the trend lines are actually close to unity, indicating the ^{14}C performance measure and maximum annual dose from ^{14}C tend to increase proportionally with the initial inventory of ^{14}C.

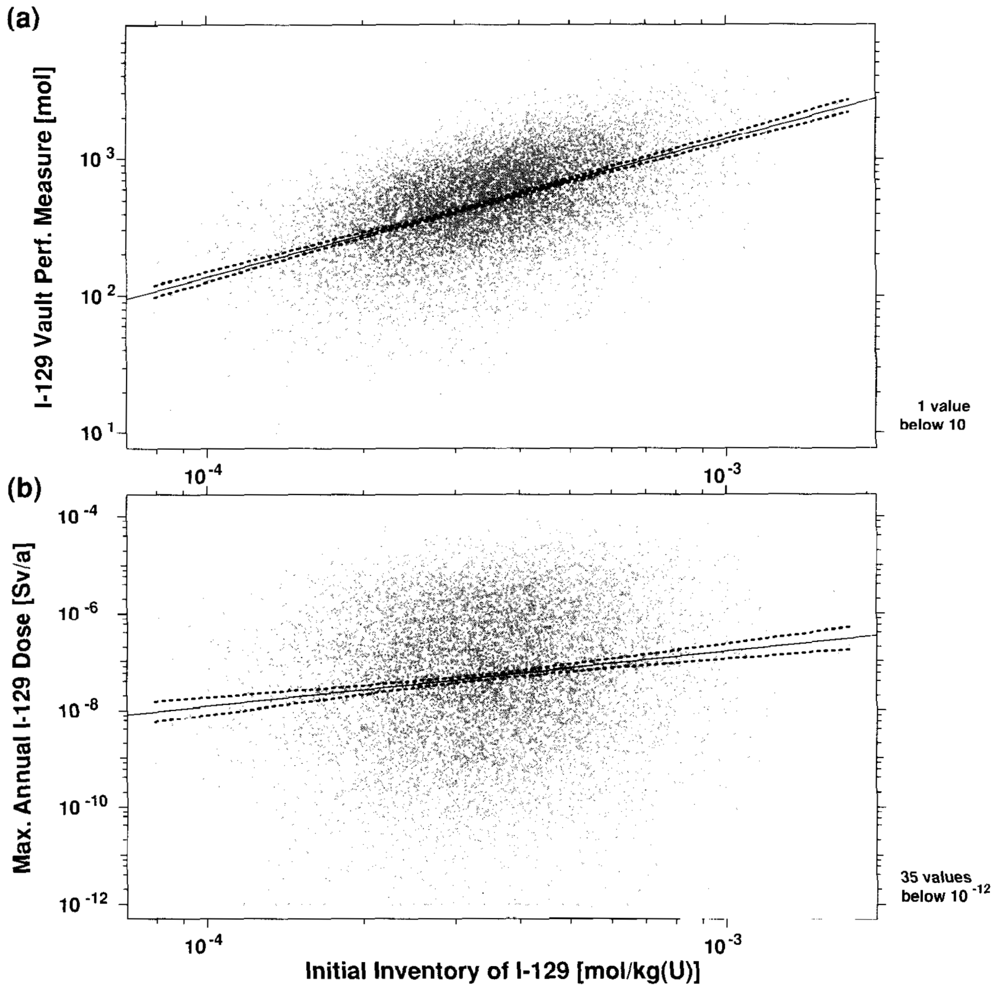


FIGURE E-3: Effect of the Initial Inventory of ^{129}I

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the initial inventory of ^{129}I in used fuel. The vertical axes are

(a) the vault performance measure for ^{129}I, defined as the total estimated amount of ^{129}I released from the vault up to 10^5 a; and

(b) the maximum annual dose estimate resulting from ^{129}I up to 10^5 a.

Correlation coefficients for the trend lines are 0.53 for the vault performance measure and only 0.13 for the maximum ADE, indicating that parameters for the geosphere and biosphere models contribute additional variability. The slopes of the trend lines are close to unity, indicating the ^{129}I performance measure and maximum annual dose from ^{129}I tend to increase proportionally with the initial inventory of ^{129}I.

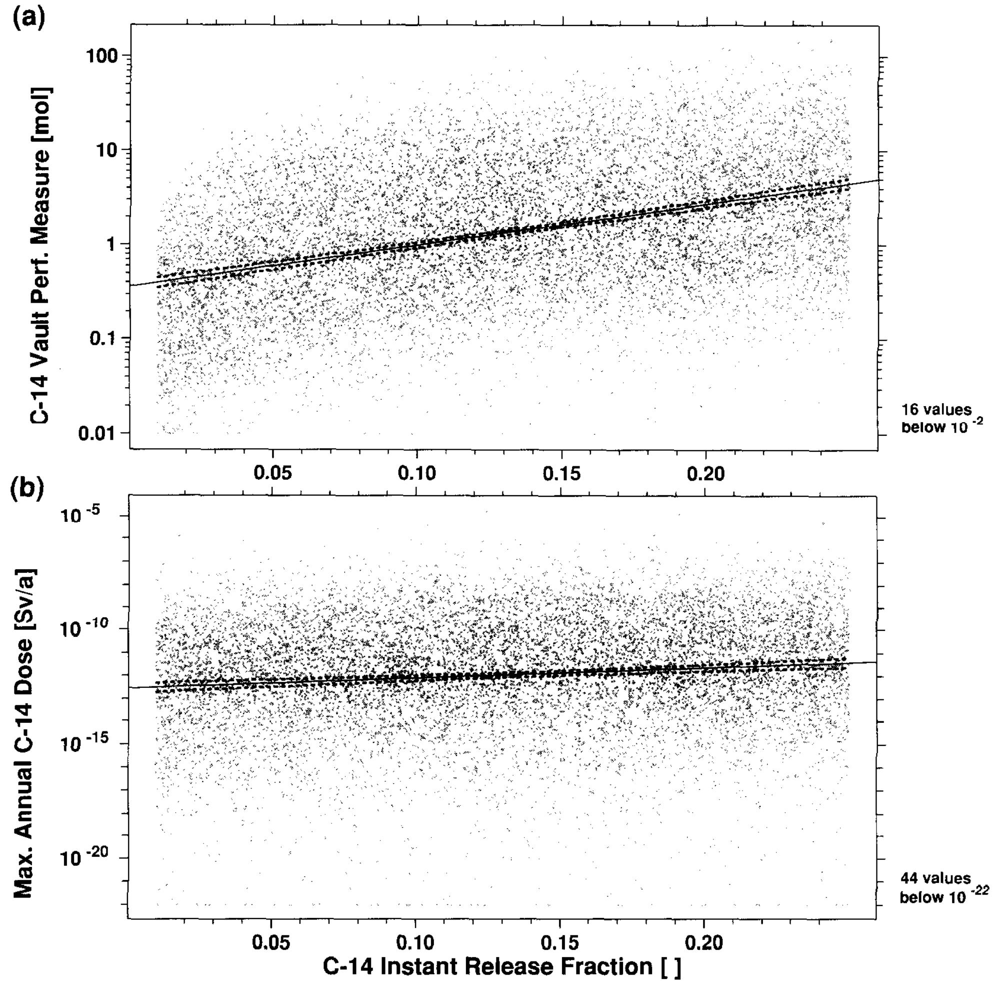


FIGURE E-4: Effect of the Instant-Release Fraction for ^{14}C

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the instant-release fraction (a dimensionless parameter) of ^{14}C in used fuel. The vertical axes are

(a) the vault performance measure for ^{14}C up to 10^5 a, and

(b) the maximum annual dose estimate from ^{14}C up to 10^5 a.

The correlation coefficients for the trend lines are 0.42 for the vault performance measure and only 0.12 for the maximum annual dose estimate, indicating that parameters for the geosphere and biosphere models contribute additional variability. The slopes of the trend lines are close to unity, indicating the ^{14}C performance measure and maximum annual dose from ^{14}C tend to increase proportionally with the instant-release fraction for ^{14}C.

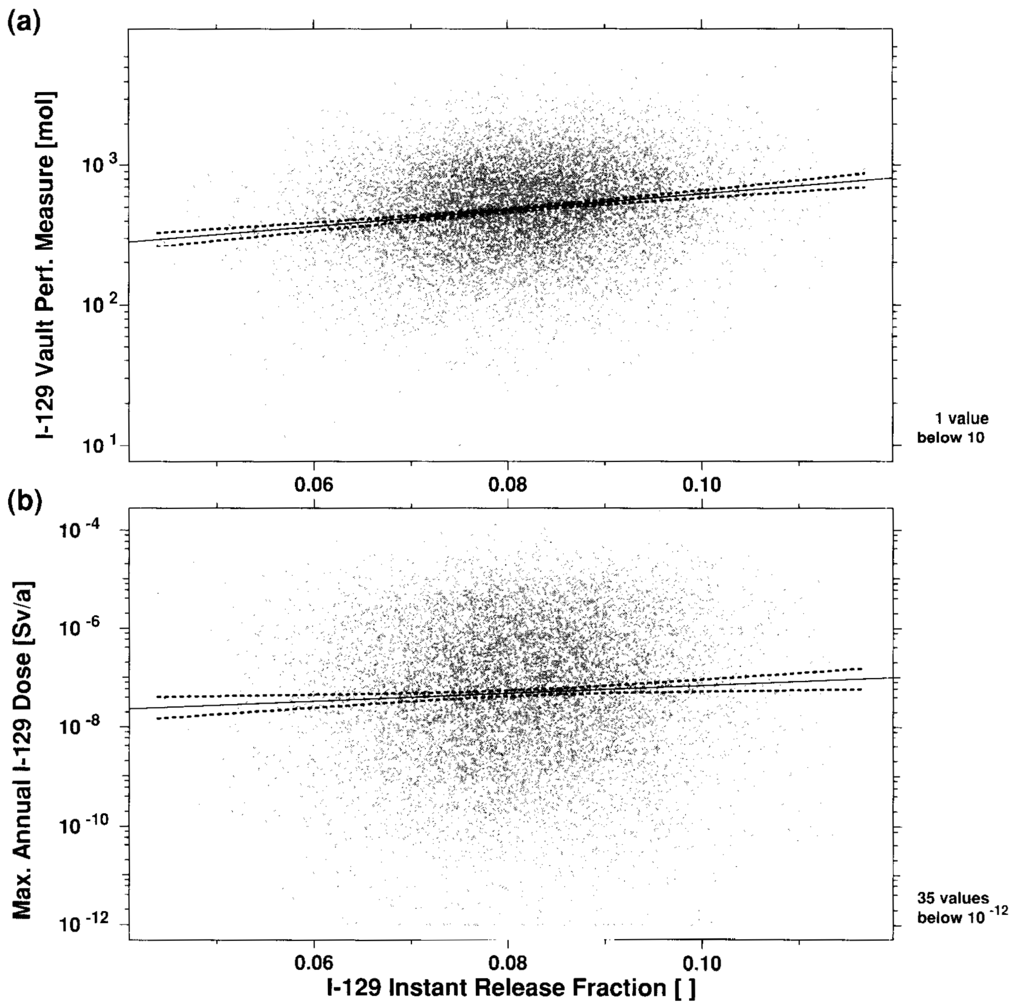


FIGURE E-5: Effect of the Instant-Release Fraction for ^{129}I

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the instant-release fraction (a dimensionless parameter) of ^{129}I in used fuel. The vertical axes are

(a) the vault performance measure for ^{129}I up to 10^5 a, and

(b) the maximum annual dose estimate resulting from ^{129}I up to 10^5 a.

The correlation coefficients for the trend lines are 0.14 for the vault performance measure and 0.08 for the maximum annual dose estimate, suggesting that parameters for the geosphere and biosphere models contribute additional variability. The slopes of the trend lines are not as close to unity as those in Figures E-2 to E-4 because the uncertainty in other parameters masks the effect (as indicated by the small values of the correlation coefficients). However, the slopes correctly indicate that the ^{129}I performance measure and maximum annual dose resulting from ^{129}I tend to increase with the instant-release fraction of ^{129}I.

The trend lines show effects that are similar to those discussed for the deterministic sensitivity analysis: their slopes (except for the line for the maximum ADE versus instant-release fraction of ^{129}I) are all near unity. This conforms with the conclusion in Section D.6 in Appendix D that the maximum ADEs and the vault performance measures are proportional to initial inventories and instant-release fractions. The slope is not quite unity for maximum ADE and instant-release fraction of ^{129}I (part (b) of Figure E-5) because the uncertainty in the other parameters is so large that it masks the effect. Nevertheless, the maximum ADE shows the expected trend; it tends to increase with increases in the instant-release fraction for ^{129}I. This trend is also obtained for the maximum ADE from all radionuclides because ^{129}I is the major contributor to dose for times up to 10^5 a.

The magnitudes of the correlation coefficients are larger for the scatter plots involving the vault performance measures, compared with the scatter plots involving the maximum ADEs. This implies that these four parameters have a greater effect on the performance measures than on the maximum ADEs. More precisely, our analysis shows that other parameters used in the geosphere and biosphere models outweigh these vault parameters in their effects on the maximum ADE.

E.4.3 EFFECTS OF THE BUFFER ANION CORRELATION PARAMETER

Figures E-6 and E-7 show the effects of the buffer anion correlation parameter for ^{14}C and ^{129}I. The results of the sensitivity analysis of the median-value simulation (Section D.6.3 in Appendix D) shows that there is a nonlinear relationship between this parameter and the vault performance measures and the maximum ADE. This nonlinear behaviour is not obvious in Figures E-6 and E-7.

The magnitudes of the correlation coefficients are larger for the scatter plots involving the vault performance measures, compared with the scatter plots involving the maximum ADEs, implying that the buffer anion correlation parameter has a greater effect on the performance measures than on the maximum ADEs. That is, other parameters used in the geosphere and biosphere models outweigh the buffer anion correlation parameter in their effects on the maximum ADE.

It is also possible to confirm that the buffer anion correlation parameter is an important parameter affecting the maximum ADE (and, therefore, it appears in Table 6-13 in the main text). This confirmation comes from examining the magnitude of the correlation coefficient for ^{129}I from the trend line for the maximum ADE resulting from ^{129}I (part (b) of Figure E-7) and from recalling that ^{129}I is the major contributor to maximum ADE for times up to 10^5 a. The value of this correlation coefficient for the buffer anion correlation parameter is 0.18, somewhat larger than the corresponding values for the initial inventory of ^{129}I (0.13; part (b) of Figure E-3) and the instant-release fraction of ^{129}I (0.08; part (b) of Figure E-5.

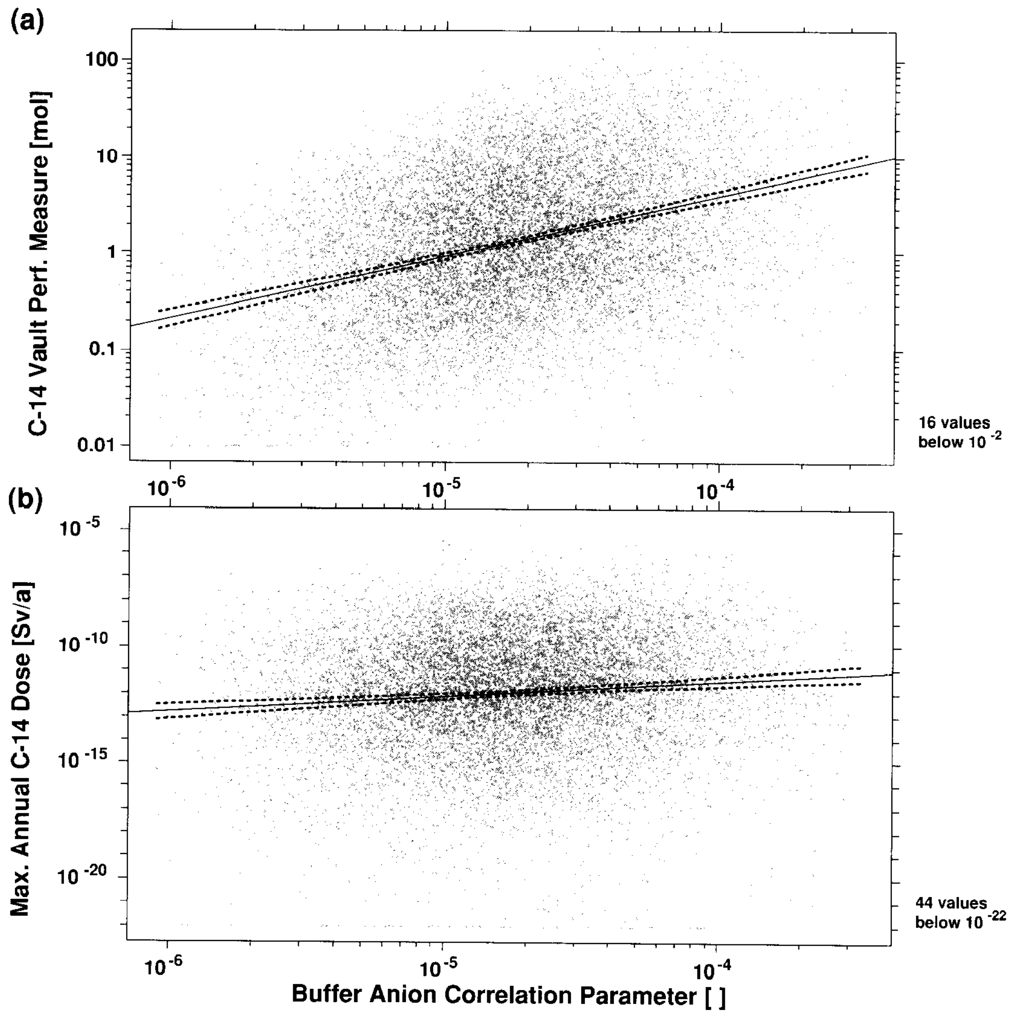


FIGURE E-6: Effect of the Buffer Anion Correlation Parameter on Results for ^{14}C

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the buffer anion correlation parameter (a dimensionless correlation parameter). The vertical axes are

(a) the vault performance measure for ^{14}C up to 10^5 a, and
(b) the maximum ADE resulting from ^{14}C up to 10^5 a.

The correlation coefficients for the trend lines are 0.36 for the vault performance measure and only 0.10 for the maximum ADE, indicating that parameters for the geosphere and biosphere models contribute additional variability.

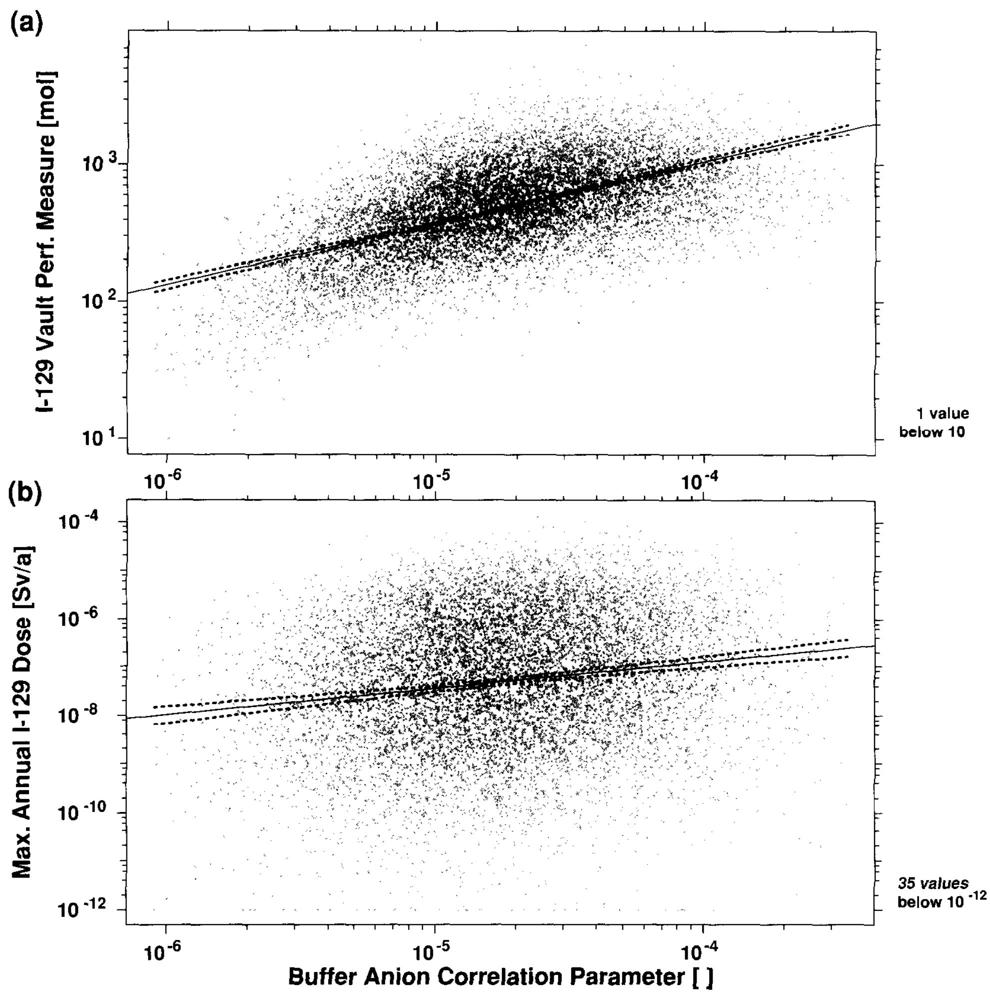


FIGURE E-7: Effect of the Buffer Anion Correlation Parameter on Results for ^{129}I

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the buffer anion correlation parameter (a dimensionless correlation parameter). The vertical axes are

(a) the vault performance measure for ^{129}I up to 10^5 a, and

(b) the maximum ADE resulting from ^{129}I up to 10^5 a.

The correlation coefficients for the trend lines are 0.56 for the vault performance measure and only 0.18 for the maximum ADE, indicating that parameters for the geosphere and biosphere models contribute additional variability.

E.4.4 EFFECTS OF PROPERTIES OF THE SURROUNDING ROCK

Figures E-8 and E-9 show the effects of the tortuosity of the lower rock zone on results for ^{14}C and ^{129}I, Figures E-10 and E-11 show corresponding effects of the groundwater velocity scaling factor.

The results of the sensitivity analysis of the median-value simulation have shown that these two parameters have complex effects because they change the time dependence of estimated releases from the vault (Section D.6.4 in Appendix D). They also have strong effects on the maximum ADEs to 10^5 a because they further act to delay contaminant transport through the geosphere (Sections D.7.3 and D.7.6 in Appendix D).

For the tortuosity of the lower rock zone, the magnitudes of the correlation coefficients are greater for the scatter plots involving the maximum ADEs, compared with the scatter plots involving the vault performance measures.

For the groundwater velocity scaling factor, the same pattern occurs for ^{14}C, but ^{129}I shows the opposite pattern. This difference is attributed to the relatively short half-life of ^{14}C (discussed previously in in Section D.7 in Appendix D). That is, the vault performance measures for ^{14}C and ^{129}I tend to be greater for larger scaling factors because more of the radionuclides are drawn out of the vault. However, the effect of greater scaling factors on estimated dose is more complex: doses tend to be larger because the radionuclides arrive earlier (more important for short-lived ^{14}C than ^{129}I), but doses are also attenuated because more uncontaminated water can reach the well, and less of the contaminant plume moving up LD1 will be captured.

It is also possible to confirm that the tortuosity of the lower rock zone is an important parameter affecting the maximum ADE (and, therefore, it appears in Table 6-13 in the main text). This confirmation comes from examining the magnitude of the correlation coefficient for ^{129}I for the maximum ADE from ^{129}I (parts (b) of Figures E-9 and E-11) and recalling that ^{129}I is the major contributor to the maximum ADE for times up to 10^5 a. The value of this correlation coefficient for the tortuosity of the lower rock zone is -0.55, greater (in absolute magnitude) than all other related correlation coefficients.

The groundwater velocity scaling factor is less important. Its correlation coefficient is 0.12, one of the largest values observed for ^{129}I but much less than the correlation coefficient for tortuosity.

E.5 SENSITIVITY ANALYSIS OF THE GEOSPHERE MODEL

E.5.1 IMPORTANT PARAMETERS OF THE GEOSPHERE MODEL

The screening of parameters from the probabilistic simulations of the system model has identified six important parameters used in the geosphere model and its linkage with the biosphere model (Table 6-13 in the main text). They are

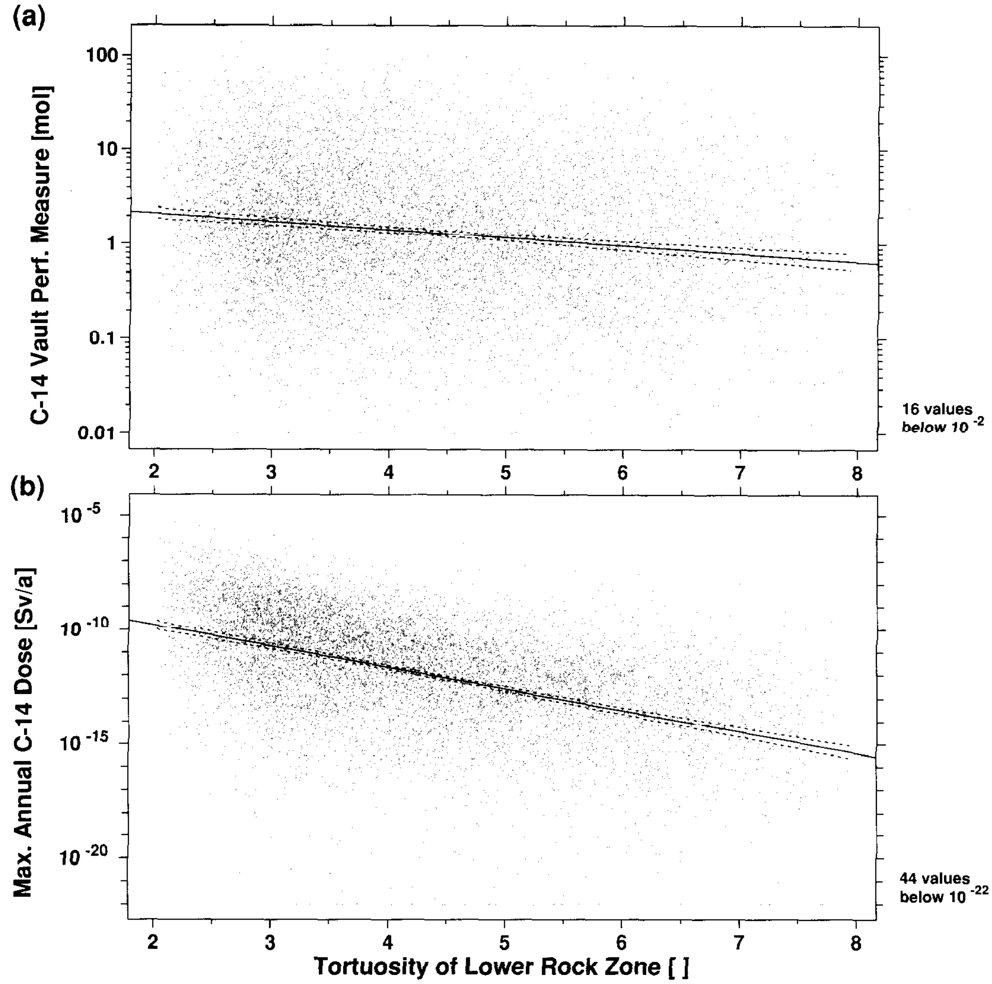


FIGURE E-8: Effect of the Tortuosity of the Lower Rock Zone on Results for ^{14}C

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the tortuosity of the lower rock zone (tortuosity is a measure of the increased distance for diffusive transport resulting from the winding nature of the interconnected aqueous pathway; it is a dimensionless parameter). The vertical axes are

(a) the vault performance measure for ^{14}C up to 10^5 a, and
(b) the maximum ADE resulting from ^{14}C up to 10^5 a.

The correlation coefficients for the trend lines are -0.12 for the vault performance measure and -0.45 for the maximum ADE. This increase (in absolute value) arises because the tortuosity of the lower rock zone is also an important factor in the geosphere model.

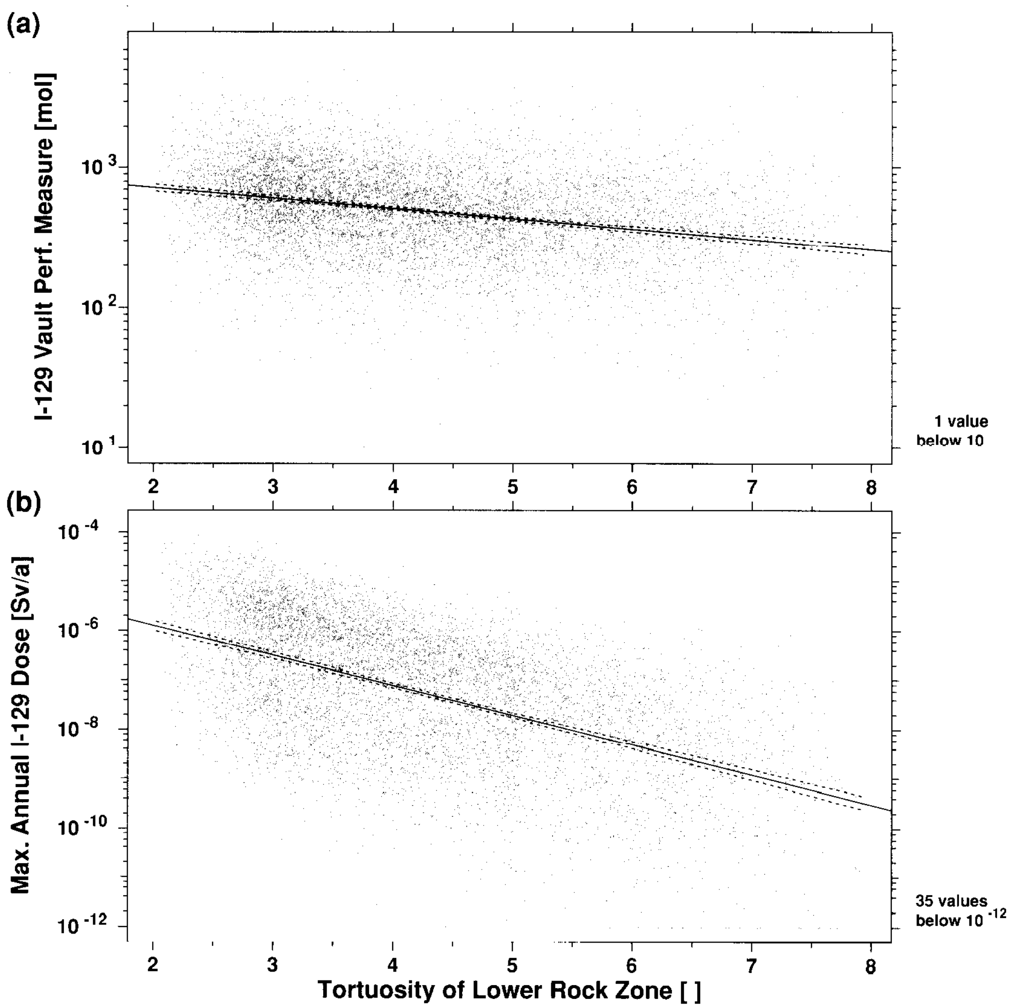


FIGURE E-9: Effect of the Tortuosity of the Lower Rock Zone on Results for ^{129}I

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the tortuosity of the lower rock zone (a dimensionless parameter). The vertical axes are

(a) the vault performance measure for ^{129}I up to 10^5 a, and

(b) the maximum ADE resulting from ^{129}I up to 10^5 a.

The correlation coefficients for the trend lines are -0.28 for the vault performance measure and -0.55 for the maximum ADE. This increase (in absolute value) arises because the tortuosity of the lower rock zone is also an important factor in the geosphere model.

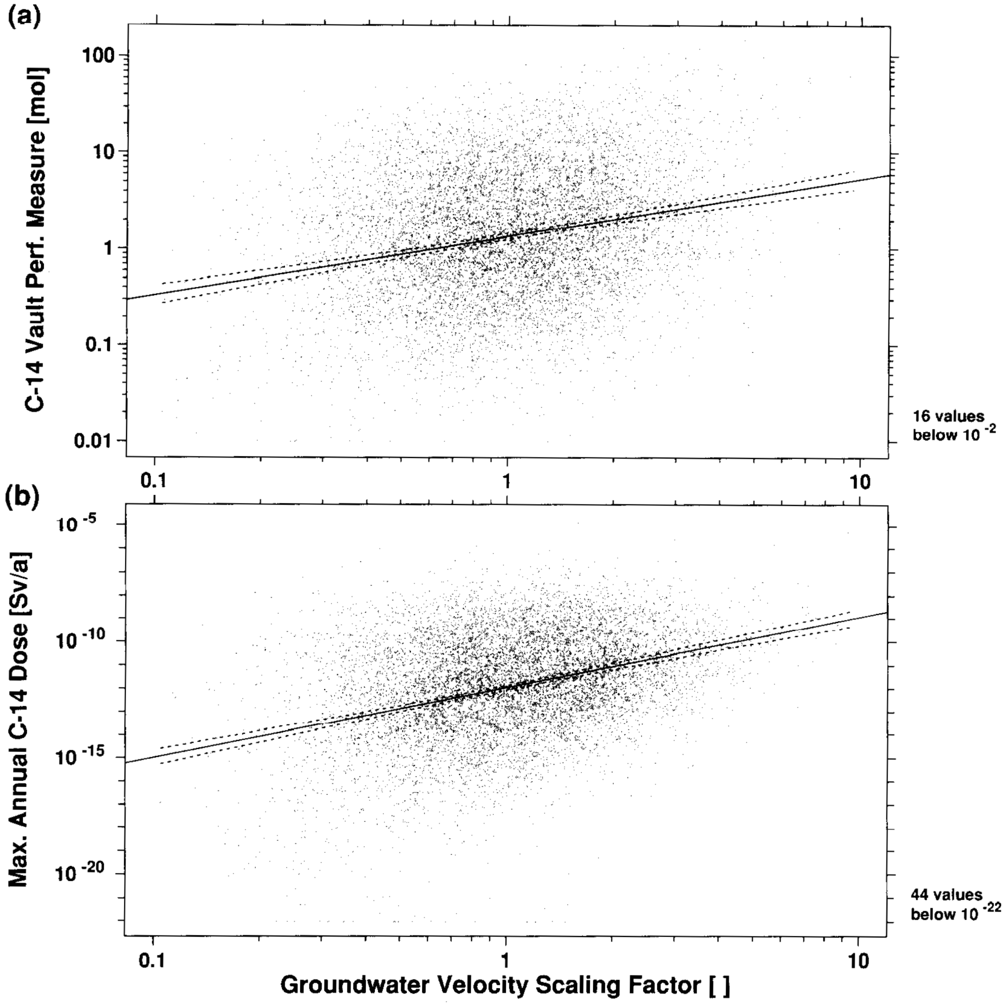


FIGURE E-10: Effect of the Groundwater Velocity Scaling Factor on Results for ^{14}C

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the groundwater velocity scaling factor (a dimensionless parameter). The vertical axes are

(a) the vault performance measure for ^{14}C up to 10^5 a, and
(b) the maximum ADE resulting from ^{14}C up to 10^5 a.

The correlation coefficients for the trend lines are 0.25 for the vault performance measure and 0.36 for the maximum annual dose estimate. This increase arises because the groundwater velocity scaling factor is also an important factor in the geosphere model. For the reference disposal system, greater values of the groundwater velocity scaling factor tend to produce larger maximum ADEs for ^{14}C because larger quantities are more likely to reach the biosphere before its undergoes radioactive decay.

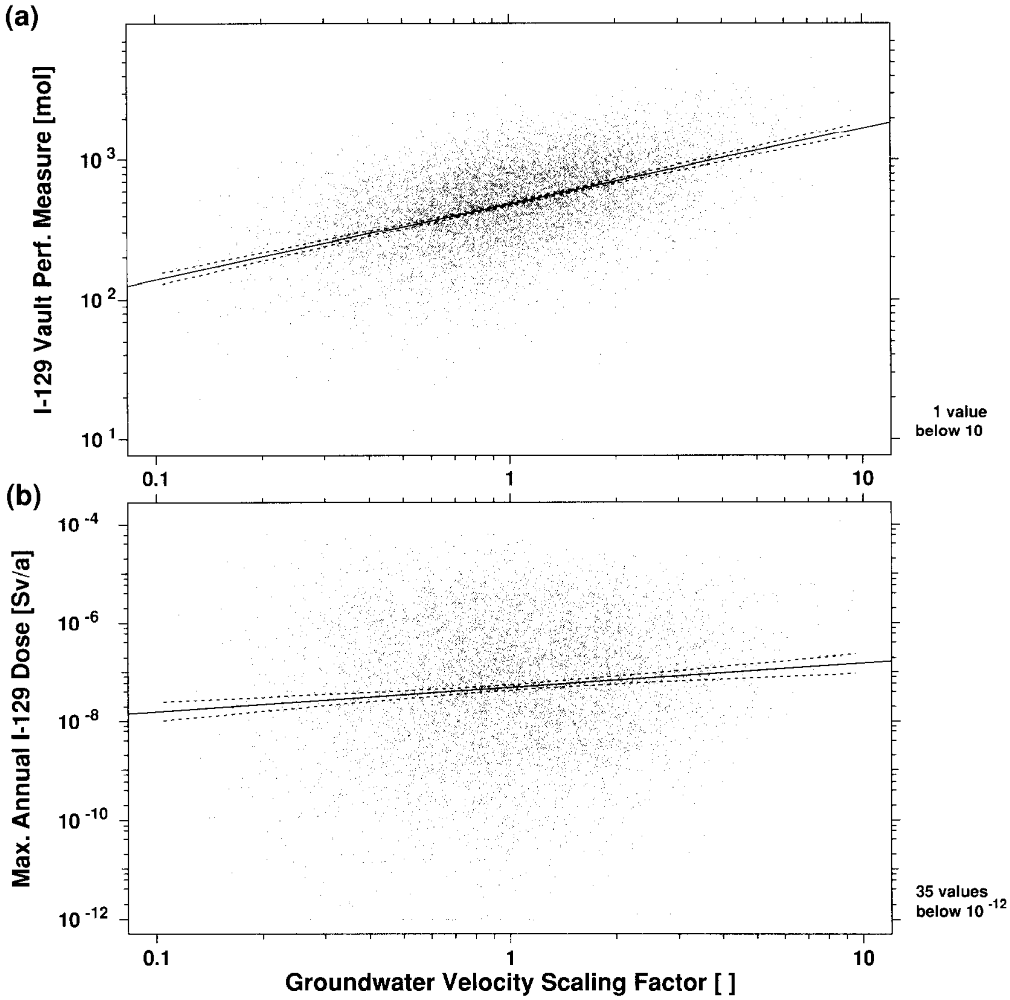


FIGURE E-11: Effect of the Groundwater Velocity Scaling Factor on Results for ^{129}I

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the groundwater velocity scaling factor (a dimensionless parameter). The vertical axes are

(a) the vault performance measure for ^{129}I up to 10^5 a, and
(b) the maximum ADE resulting from ^{129}I up to 10^5 a.

The correlation coefficients for the trend lines are 0.46 for the vault performance measure and 0.12 for the maximum ADE. This decrease arises because the groundwater velocity scaling factor is also an important factor in the geosphere model. For the reference disposal system, greater values of the groundwater velocity scaling factor tend to produce larger maximum ADEs for ^{129}I. The effect is less pronounced for ^{129}I than for ^{14}C (Figure E-11) because of ^{129}I has a much longer half-life.

- Tortuosity of the lower rock zone (a measure of the increase in the effective distance for transport by diffusion resulting from the winding nature of the interconnected aqueous pathway);

- Groundwater velocity scaling factor (describes uncertainty in groundwater velocities in the transport network and used in such a way that groundwater velocities in all segments are increased or decreased by the same amount);

- Free-water diffusion coefficient for iodine (describing ^{129}I transport by diffusion in water);

- The retardation factor of iodine in compacted organic lake sediment (equal to the ratio of the groundwater velocity to the transport velocity of iodine in moving water; its minimum value is one, meaning that the contaminant moves at the same velocity as groundwater, whereas a value greater than unity means that the contaminant is moves slower than the groundwater);

- The thickness of compacted lake sediment at Boggy Creek South; and

- The depth of the well (overburden wells are relatively shallow, extending only into the overburden that overlies the rock of the geosphere; bedrock wells are deeper, and we assume that they always intersect fracture zone LD1).

These parameters are important in the probabilistic simulations, in the sense that variations from their 0.01 to 0.99 quantiles result in significant changes to the maximum ADEs to humans. From the results in Table 6-13 in the main text it is clear that the effects of the first three parameters are considerably stronger than the effects of the last three.

Another fractional factorial screening study was directed at the geosphere performance measures for ^{129}I and ^{14}C. The geosphere performance measure for ^{129}I is defined as the total amount of ^{129}I that leaves the geosphere divided by the total amount of ^{129}I that enters the geosphere, over 10^5 a. A similar performance measure is defined for ^{14}C. This study identified two additional parameters that had moderate to weak effects on the geosphere performance measures (Table E-1):

- the free-water diffusion coefficient for carbon, and

- the retardation factor of carbon in compacted organic lake sediment.

One other parameter listed in Table E-1, the thickness of overburden at Boggy Creek South, has very weak effects and is not discussed further.

Only two of the eight parameters listed above are not identified in sensitivity analysis of the median-value simulation (Sections 6.3.3 in the main text and D.5 to D.8 in Appendix D): the retardation factors for iodine and carbon in compacted organic lake sediment. In the median-value simulation, we assume that the well (and not the lake) is the source of drinking water for the critical group. As a consequence, parameters describing processes in the lake (including retardation factors) are relatively unimportant in the median-value simulation.

Scatter plots are used to show the effects of the important parameters. The effects are shown for the geosphere performance measures for ^{129}I and ^{14}C, and the maximum ADE up to 10^5 a from ^{129}I and ^{14}C. Each plot includes a trend line and its associated 95% confidence bands. The trend line (or regression line) is the least-squares fit (Section A.4.3.2 in Appendix A) to the logarithm of the parameter values and the logarithm of the estimated variables. The associated 95% confidence bands put bounds on the location of this trend line (Section A.4.3.3 in Appendix A).

Correlation coefficients measure the extent to which the data fits the regression line (Section A.4.3.2). The degree of spread of data points about the trend line is a reflection of the effects of the range of possible values of the other parameters. Correlation coefficients vary from +1 to -1: values near +1 or -1 indicate a linear relationship between the estimated variable and the parameter, whereas values near zero imply no such relationship exists.

Table E-5 shows the correlation coefficients calculated for the eight parameters listed above. The results in the table show that

- For most parameters, the correlation coefficients are closer to +1 or -1 for the geosphere performance measures than for the maximum ADE. This occurs because of the added variability of the vault and biosphere models that affect the ADEs.

- The first three parameters on the list have the largest correlation coefficients for the maximum ADE from ^{129}I. This is fully consistent with the relative importance of these same parameters to the maximum ADE from all radionuclides (Table 6-13 in the main text) and follows because ^{129}I is the major contributor to dose for times up to 10^5 a.

The effects that these parameters have on the mean of the maximum ADEs are similar to the effects on the dose estimate from the median-value simulation, described in Section D.7 in Appendix D. In particular, the tortuosity of the lower rock zone is again an important parameter, followed by the groundwater velocity scaling factor. However, the results here indicate that the tortuosity is clearly the most important parameter. In fact, the variability in maximum estimated dose is more the result of the uncertainty in the tortuosity than the uncertainty in all other parameters.

E.5.2 EFFECTS OF TORTUOSITY OF THE LOWER ROCK ZONE

Uncertainty in the tortuosity of the lower rock zone is the largest source of variability in the maximum ADE and the geosphere performance measures for ^{14}C and ^{129}I. The ADEs up to 10^5 a are also much smaller when the tortuosity is large.

The tortuosity of the lower rock zone controls the transport of contaminants across the diffusion barrier of the lower rock zone, including rock within the waste exclusion distance that isolates the vault rooms from fracture zone LD1.

TABLE E-5

CORRELATION COEFFICIENTS SUMMARIZING EFFECTS OF EIGHT IMPORTANT GEOSPHERE PARAMETERS*

Parameter	Correlation Coefficients			
	Geosphere Performance Measure for		Maximum Annual Dose to 10^5 a from	
	^{14}C	^{129}I	^{14}C	^{129}I
Tortuosity of the lower rock zone	-0.66	-0.86	-0.45	-0.55
Groundwater velocity scaling factor	0.53	0.15	0.36	0.12
Free-water diffusion coefficient (iodine)	**	0.23	**	0.13
Thickness of compacted lake sediment at Boggy Creek South***	-0.12	-0.08	-0.07	-0.04
Depth of the well	0.03	-0.03	0.08	0.06
Retardation factor of iodine in compacted organic lake sediment***	**	-0.20	**	-0.11
Retardation factor of carbon in compacted organic lake sediment***	-0.28	**	-0.15	**
Free-water diffusion coefficient (carbon)	0.18	**	0.14	**

* These correlation coefficients are calculated from a set of 10 000 randomly sampled simulations; they reflect the spread of results about the trend lines shown in the figures and discussed in Sections E.5.2 to E.5.4. A correlation coefficient equal to zero implies that there is no relationship between the estimated variable and the parameter and that there is a wide spread of plotted points about the trend line. Correlation coefficients of +1 or -1 imply that there is a linear relationship between these parameters.
The results of this table indicate the two parameters with largest effects are the tortuosity of the lower rock zone and the groundwater velocity scaling factor.

** The parameters are specific to another radionuclide.

*** Calculation of the geosphere performance measure for these parameters considers the amounts of ^{14}C and ^{129}I that exit from the compacted lake sediment. That is, the "end" of the geosphere is taken to be the top of the compacted lake sediment. For all other parameters (and in Section E.3), the calculation of the geosphere performance measure assumes that the end of the geosphere is the top of the overburden. Figure E-19 (and others) illustrates results using both the top of the compacted lake sediment and the top of the overburden.

The sensitivity of the geosphere model to the tortuosity of the lower rock zone is clearly evident when observing the performance of the geosphere model alone, eliminating the variability resulting from the vault and biosphere models. Figure E-12 shows two scatter plots where the geosphere performance measure for ^{14}C and the maximum ADE to 10^5 a resulting from ^{14}C are plotted against the tortuosity. Figure E-13 shows similar results for ^{129}I. The two figures show that the variation of the tortuosity causes a variation of 5 or more orders of magnitude in the geosphere performance measures and maximum ADEs. The trend lines indicate that the performance measure and maximum ADEs tend to decrease as the tortuosity increases. A similar trend is observed in the sensitivity analysis of the median-value simulation (Section D.7.6 in Appendix D).

Figure 6-21 (Section 6.5.5 in the main text) shows a scatter plot of maximum ADE from ^{129}I at 10^4 and 10^5 a and tortuosity of the lower rock zone. (Parts (b) of Figures 6-21 and E-13 are identical.) There is more variability at 10^4 a than 10^5 a because the leading edge of ^{129}I discharges is just starting (and is more variable) at the earlier time. That is, uncertainty in the tortuosity of the lower rock zone results in more variability in the ADE at early times that at late times because the tortuosity is effective only in delaying the movement of ^{129}I.

Tortuosity has been assigned the triangular probability density function (Davison et al. 1994) shown in Figure E-14, with a range from 2.0 to 8.0, a most probable value (mode) of 3.0 and a median value of 4.1. This variation of tortuosity results in the large variations shown in Figures E-12, E-13 and 6-21 (upon which is superimposed the effects of the other parameters). The tortuosity of the lower rock zone is important because of

- the sensitivity of transport by diffusion to this parameter, and
- the effects of its range of possible values.

The distribution of values for this parameter reflects the uncertainty in characterizing the diffusion properties of the lower rock zone. Section E.7 examines how some changes to the PDF for the tortuosity of the lower rock zone would affect ADEs.

E.5.3 EFFECTS OF THE GROUNDWATER VELOCITY SCALING FACTOR

The groundwater velocity scaling factor is applied uniformly to the entire network of segments simulated in the geosphere model (Section 5.4 in the main text) and reflects the uncertainty in our knowledge of the groundwater flow system for the reference disposal system over the time period of the simulations. The discussion in Section D.7.3 in Appendix D shows that the groundwater velocity scaling factor affects

- The drawdown of hydraulic heads caused by the well, which influences groundwater flow velocities toward the well and the amount of diluting water captured by the well;
- The capture of contaminants by a well that is sufficiently deep to intersect fracture zone LD1;

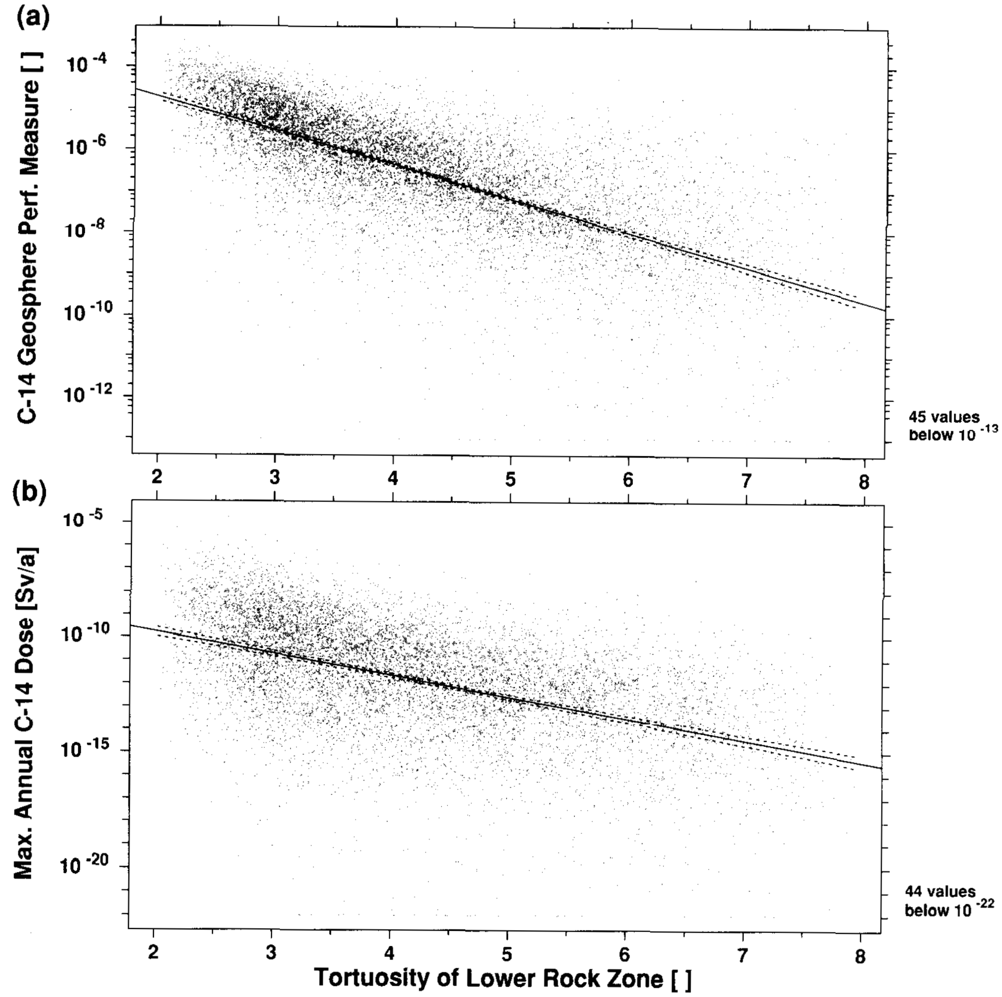


FIGURE E-12: Effect of the Tortuosity of the Lower Rock Zone on Results for ^{14}C

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the tortuosity of the lower rock zone (a dimensionless parameter). The vertical axes are

(a) the geosphere performance measure for ^{14}C, defined as the total estimated amount of ^{14}C that leaves the geosphere divided by the total amount of ^{14}C that enters the geosphere, over 10^5 a; and
(b) the maximum ADE from ^{14}C up to 10^5 a.

The correlation coefficients for the trend lines are -0.66 in part (a) and -0.45 in part (b). These plots *confirm that the tortuosity of the lower rock zone* has a very large influence on the geosphere performance measure for ^{14}C and the maximum annual dose resulting from ^{14}C. Larger values of tortuosity generally yield smaller performance measures and ADEs.

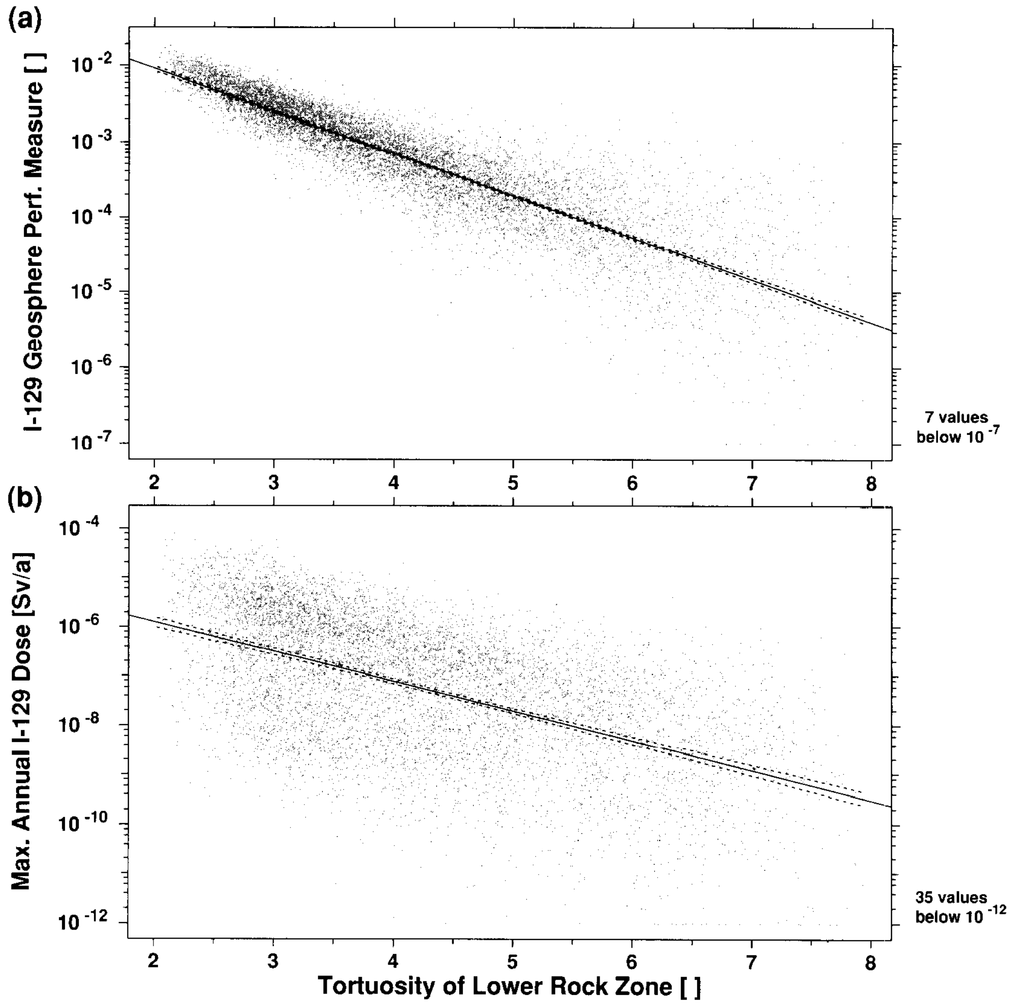


FIGURE E-13: Effect of the Tortuosity of the Lower Rock Zone on Results for ^{129}I

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the tortuosity of the lower rock zones (a dimensionless parameter). The vertical axes are

(a) the geosphere performance measure for ^{129}I, defined as the total estimated amount of ^{129}I that leaves the geosphere divided by the total amount of ^{129}I that enters the geosphere, over 10^5 a; and

(b) the maximum ADE from ^{129}I up to 10^5 a.

The correlation coefficients for the trend lines are -0.86 in part (a) and -0.55 in part (b). These plots confirm that the tortuosity of the lower rock zone has a very large influence on the geosphere performance measure for ^{129}I and the maximum annual dose from ^{129}I. Larger values of tortuosity generally yield smaller performance measures and ADEs.

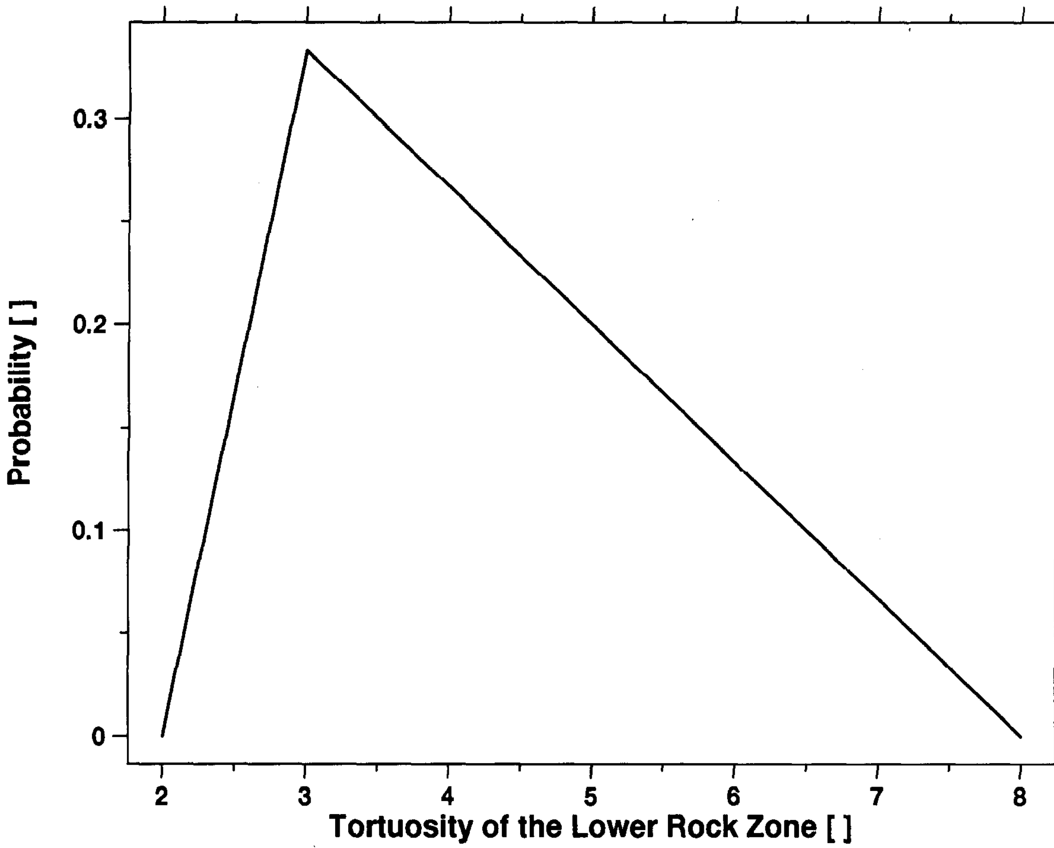


FIGURE E-14: Probability Density Function for Tortuosity

The tortuosity of the lower rock zone is characterized by a triangular PDF, with values ranging from 2.0 to 8.0. The most probable value, or mode, of the distribution is 3.0, its median is 4.1, and its mean (average) is 4.33.

- The release of contaminants from the vault through changes to the mass transfer coefficients; and

- The convective transport in moving groundwater of contaminants in all segments, including those within the waste exclusion distance.

The effects are not readily observed in the randomly sampled simulations, but the probabilistic sensitivity analysis indicates its net effect: lower values of the groundwater velocity scaling factor generally lead to smaller estimates of annual dose.

Figure E-15 shows two scatter plots where, the geosphere performance measure for ^{14}C and the maximum ADE to 10^5 a from ^{14}C are plotted against the groundwater velocity scaling factor. Figure E-16 shows similar results for ^{129}I. These figures show

- the effects of the groundwater velocity scaling factor are much less important than the effects of the tortuosity of the lower rock zone,

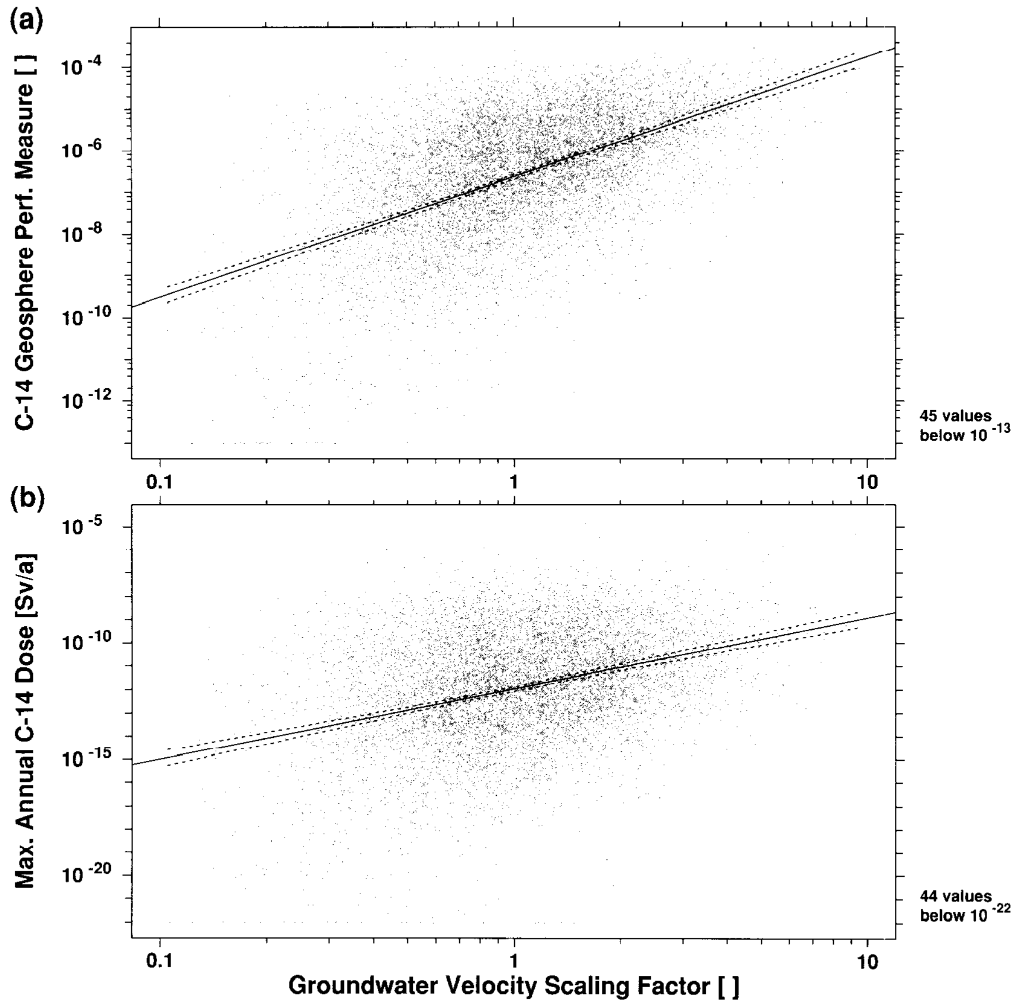


FIGURE E-15: Effect of the Groundwater Velocity Scaling Factor on Results for ^{14}C

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the groundwater velocity scaling factor (a dimensionless parameter). The vertical axes are

(a) the geosphere performance measure for ^{14}C over 10^5 a, and
(b) the maximum ADE from ^{14}C up to 10^5 a.

The correlation coefficients for the trend lines are 0.53 in part (a) and 0.36 in part (b). These plots show that higher groundwater velocities generally result in greater geosphere performance measures for ^{14}C and larger maximum annual doses from ^{14}C.

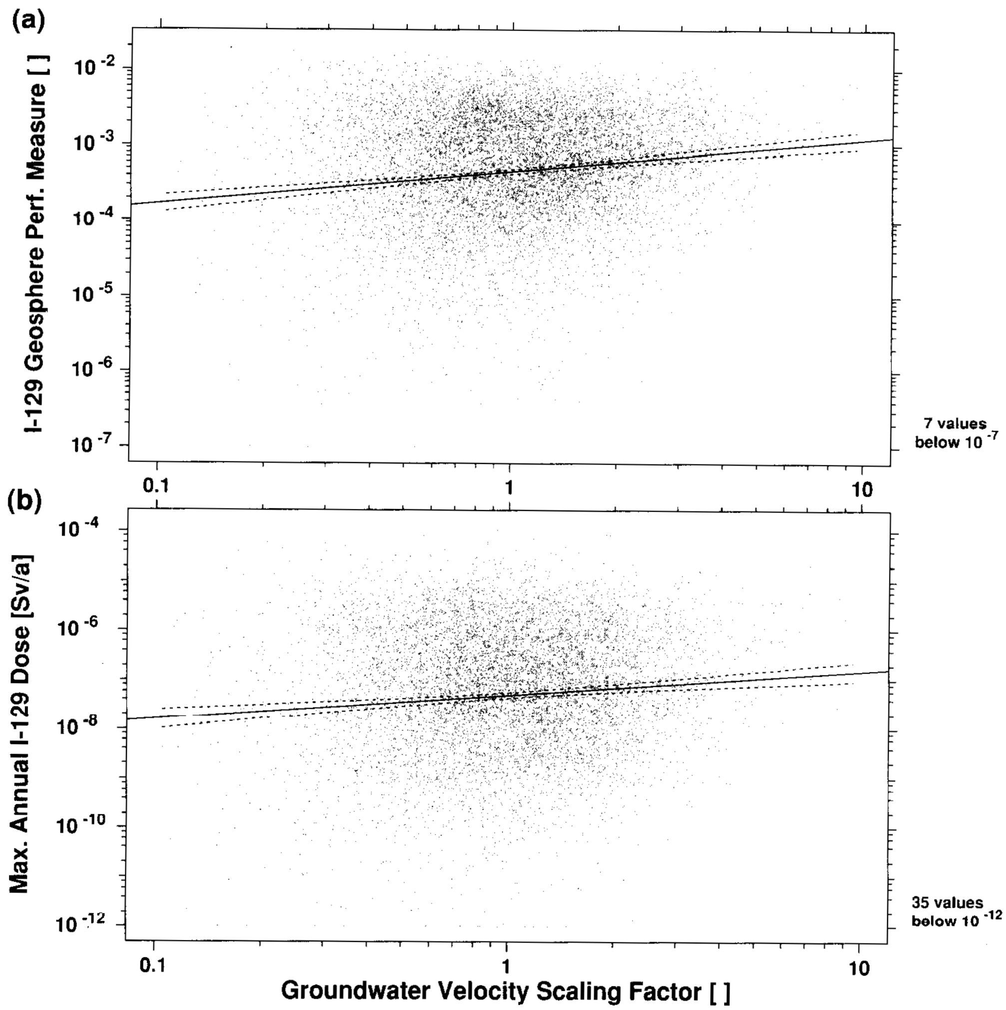


FIGURE E-16: Effect of the Groundwater Velocity Scaling Factor on Results for ^{129}I

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the groundwater velocity scaling factor (a dimensionless parameter). The vertical axes are

(a) the geosphere performance measure for ^{129}I over 10^5 a, and

(b) the maximum ADE from ^{129}I up to 10^5 a.

The correlation coefficients for the trend lines are 0.15 in part (a) and 0.12 in part (b). These plots show that higher groundwater velocities generally result in greater geosphere performance measures for ^{129}I and larger maximum annual doses from ^{129}I.

- the trends are stronger for ^{14}C than for ^{129}I, and

- The maximum ADE to 10^5 a and the geosphere performance measures for ^{14}C and for ^{129}I all tend to increase with larger values of the groundwater velocity scaling factor.

Figure E-17 shows separately the effects of the scaling factor on two groups of simulations: in one group the source of domestic water is the well and in the other it is the lake. To isolate an effect of the well, we use a modified geosphere performance measure in part (a) of the figure. The original geosphere performance measure is the total amount of ^{129}I that leaves the geosphere divided by the total amount of ^{129}I that enters the geosphere, over 10^5 a. The modified geosphere performance measure is the amount of ^{129}I that leaves from the well divided by the total amount of ^{129}I that enters the geosphere, over 10^5 a. Thus parts (a) and (b) of the figure deal with the amount of ^{129}I that is discharged to the well and to the lake. The trend lines show that the performance measure increases as the scaling factor increases for the lake simulations but decreases for the well simulations.

We attribute these different trends to the complex relationship between groundwater transport and the other parts of the disposal system. For example, the negative slope for simulations involving the well is consistent with the capture of smaller fractions of the contaminant plume as the groundwater velocity scaling factor increases (see Figure D-43 in Appendix D), whereas the positive slope for simulations involving the lake is consistent with the more rapid transport of contaminants from the disposal vault to the biosphere (Figure D-48 in Appendix D). (A plot using the original geosphere performance measure for the well simulations shows a trend similar to that for the lake because the amount of ^{129}I not captured by the well is discharged to the lake.) In the sensitivity analysis of the median-value simulation for the geosphere model (Section D.7 in Appendix D), we describe the complex interplay between the groundwater velocity scaling factor, the depth of the well and the volume of water drawn from the well (which is a function of the number of persons making up the household of the critical group). Although these effects can be observed in the median-value simulation, they are not as clearly evident in the probabilistic simulations because the variation of the other parameters obscures all but the strongest effects.

E.5.4 EFFECTS OF OTHER GEOSPHERE PARAMETERS

We discuss in this section the effects of the six other parameters:

- the free-water diffusion coefficient for iodine,

- the retardation factor of iodine in compacted organic lake sediment,

- the thickness of compacted lake sediment at Boggy Creek South,

- the depth of the well,

- the free-water diffusion coefficient for carbon, and

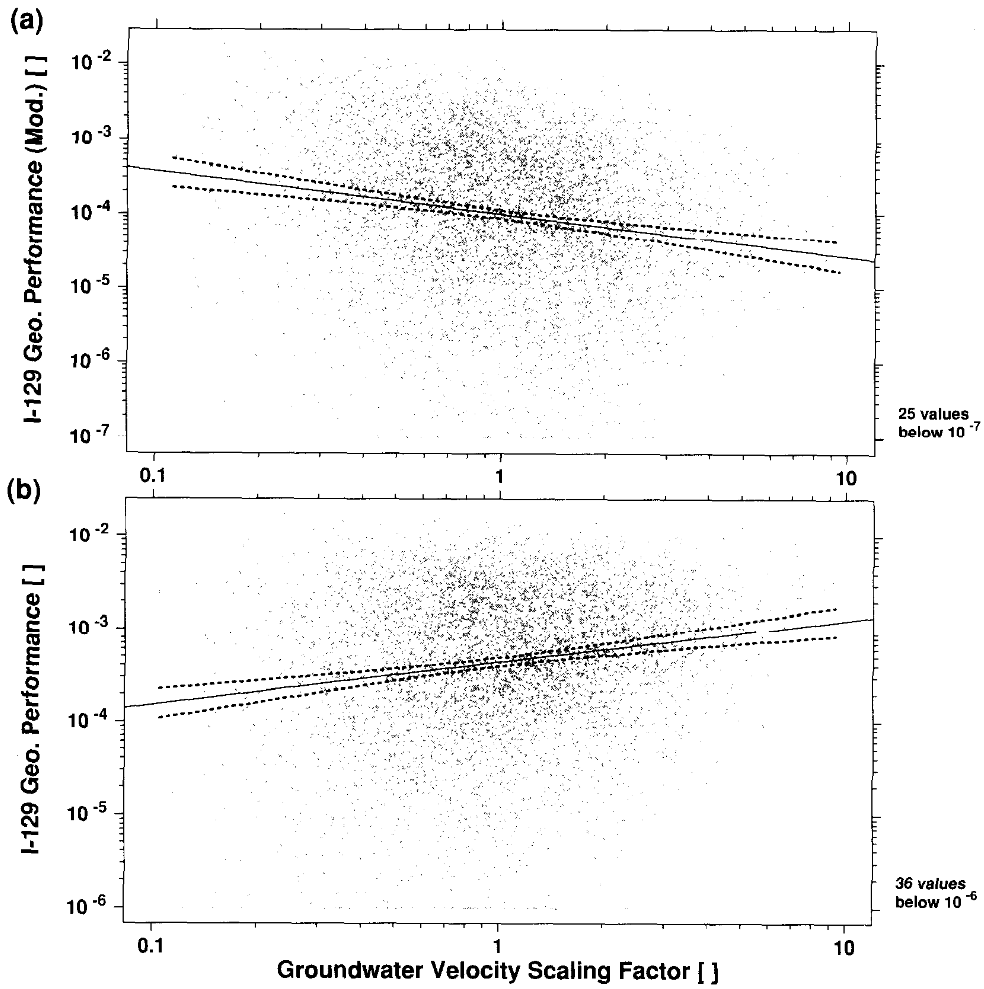


FIGURE E-17: Effects of the Groundwater Velocity Scaling Factor on Simulations Involving the Well and Lake

Each plot shows approximately 5000 data points, with the groundwater velocity scaling factor (a dimensionless parameter) on the horizontal axis. We illustrate a subtle effect of the well through the use of a modified geosphere performance measure on the vertical axis:

- Part (a) applies to approximately 5000 simulations where the well is the source of drinking water, and the modified geosphere performance measure is the amount of ^{129}I that leaves from the well divided by the total amount of ^{129}I that enters the geosphere, over 10^5 a.
- Part (b) applies to approximately 5000 simulations where the lake is the source of drinking water, and the (original) geosphere performance measure is the total amount of ^{129}I that leaves the geosphere divided by the total amount of ^{129}I that enters the geosphere, over 10^5 a.

The correlation coefficients for the trend lines are -0.16 in part (a) and 0.16 in part (b). The slopes of the two trend lines have different signs, showing opposite relationships between the groundwater velocity scaling factor and the geosphere performance measures for the well and the lake (see text).

- the retardation factor of carbon in compacted organic lake sediment.

The correlation coefficients for these parameters (Tables 6-13 in the main text, E-1 and E-5) show that the effects of these parameters are much smaller than the effects of the tortuosity of the lower rock zone and the groundwater velocity scaling factor. In general, effects can only be readily discerned using statistical tools.

Figures E-18 and E-19 show the effects of the free-water diffusion coefficients for carbon and iodine. The trend lines show the expected effect:

- the geosphere performance measures and the maximum ADEs tend to increase with greater values of the free-water diffusion coefficients, which correspond to increased rates of transport of ^{14}C and ^{129}I through the rock of the geosphere.

The effects of the retardation factors of carbon and iodine in compacted organic lake sediment are shown in Figures E-20 and E-21. The original geosphere performance measures, plotted in part (a) of the figures, show weak trends or no trends; however, the expected trends can be unraveled using the modified performance measures shown in part (b) of the figures. The slopes of the trend lines in parts (b) and (c) of Figures E-20 and E-21 indicate that

- the geosphere performance measures and the maximum ADEs tend to decrease with larger values of the retardation factors of carbon and iodine in compacted organic lake sediment, which correspond to increased delays in the transport of ^{14}C and ^{129}I.

Figures E-22 and E-23 show the effects of the thickness of compacted lake sediment at Boggy Creek South. As in the previous figures, we use modified geosphere performance measures to illustrate the weak trends. The slopes of the trend lines in parts (b) and (c) of Figures E-22 and E-23 show that

- the geosphere performance measures and the maximum ADEs tend to decrease with greater values for the thickness of the compacted lake sediment, which produces increased delays in the transport of ^{14}C and ^{129}I.

Figures E-24 and E-25 show the effects of the depth of the well. In Sections 5.4 in the main text and D.7 in Appendix D, we identify two broad clarifications of wells: overburden and bedrock wells. The former wells are relatively shallow and extend only into the overburden, whereas the latter are deeper and extend into the rock of the geosphere. We also change the location of the bedrock wells from one simulation to the next: a bedrock well is constrained to lie along the centre of the contaminant plume, such that it intersects fracture zone LD1 at the deepest possible spot. The slopes of the trend lines in Figures E-24 and E-25 show that

- the geosphere performance measure for ^{14}C and the maximum ADEs from ^{14}C and ^{129}I tend to increase with greater values of the depth of the well, whereas the geosphere performance measure for ^{129}I shows a small decrease with greater depths of the well.

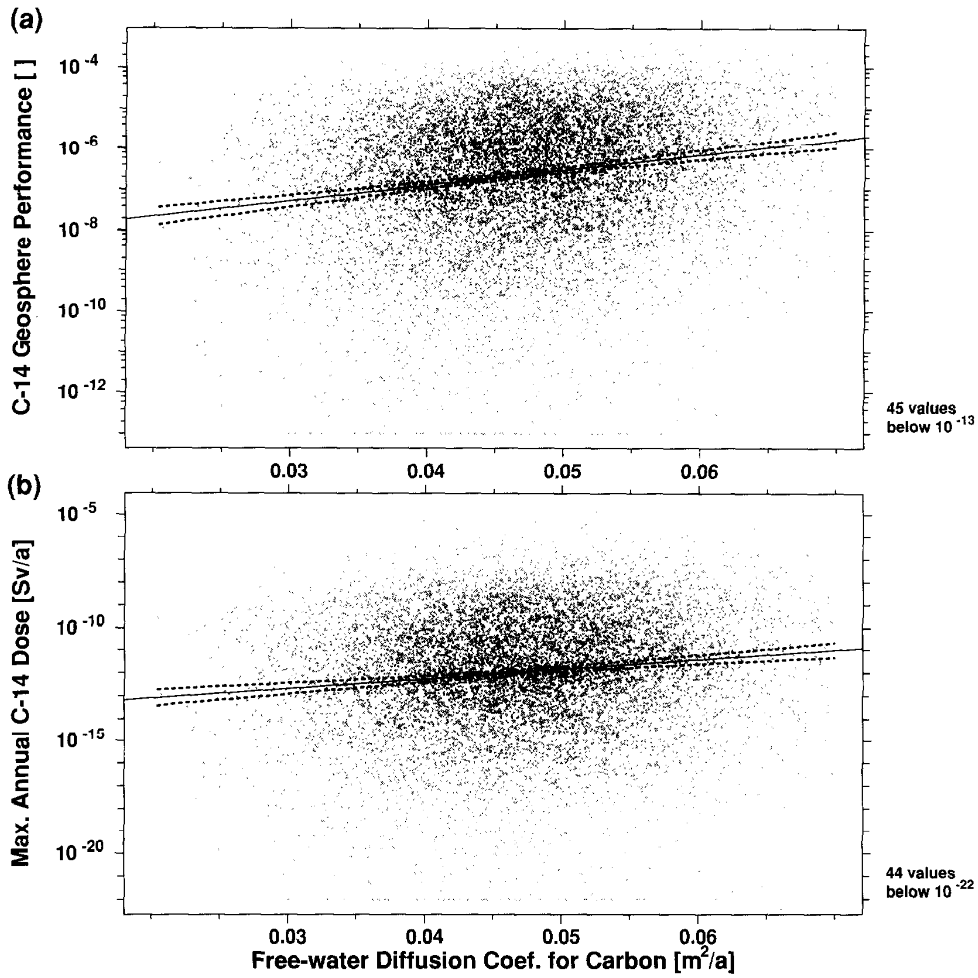


FIGURE E-18: Effect of the Free-Water Diffusion Coefficient for Carbon

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the free-water diffusion coefficient for carbon. The vertical axes are

(a) the geosphere performance measure for ^{14}C over 10^5 a; and
(b) the maximum ADE from ^{14}C up to 10^5 a.

The correlation coefficients for the trend lines are 0.18 in part (a) and 0.14 in part (b). These plots show that greater free-water diffusion coefficients for carbon generally result in greater geosphere performance measures for ^{14}C and larger maximum ADEs from ^{14}C because of the increased rate of transport of ^{14}C through the rock of the geosphere.

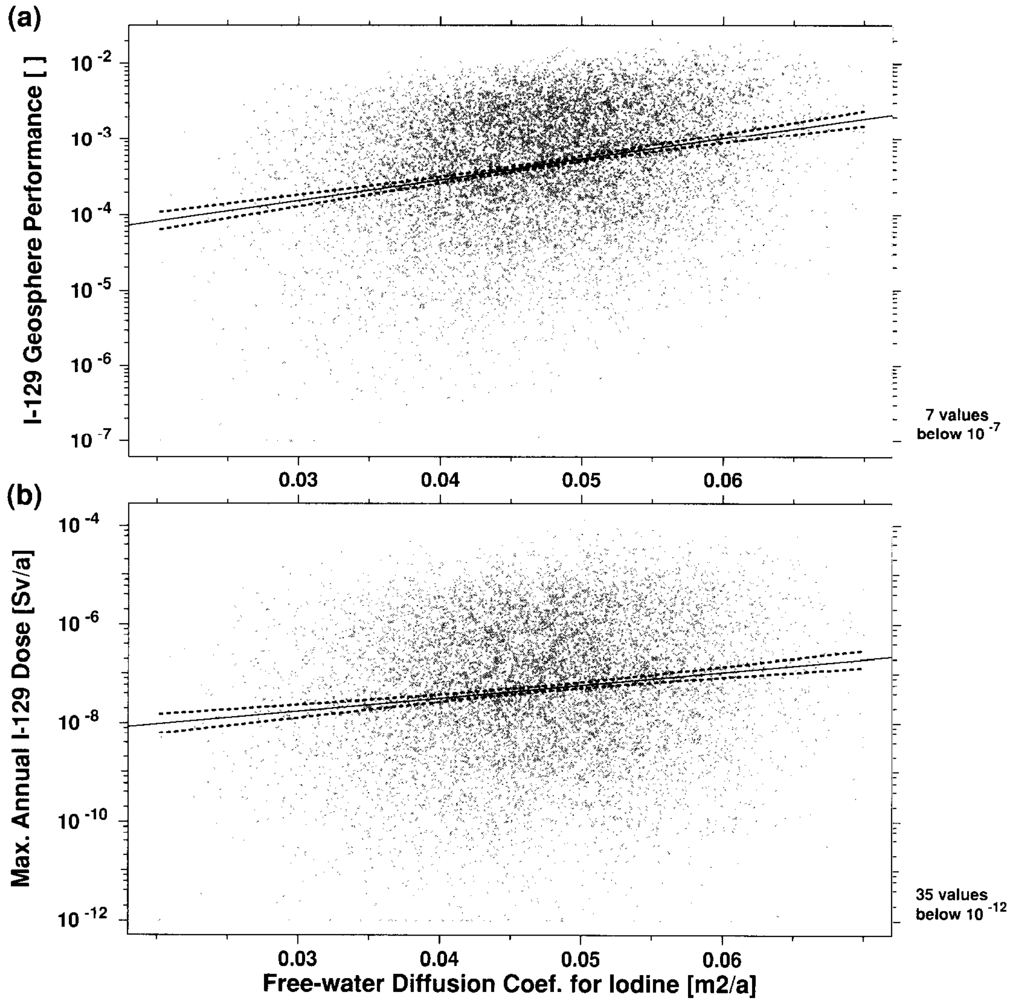


FIGURE E-19: Effect of the Free-Water Diffusion Coefficient for Iodine

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes show the free-water diffusion coefficient for carbon. The vertical axes are

(a) the geosphere performance measure for ^{129}I over 10^5 a; and
(b) the maximum ADE from ^{129}I up to 10^5 a.

The correlation coefficients for the trend lines are 0.23 in part (a) and 0.13 in part (b). These plots show that greater free-water diffusion coefficients for iodine generally result in greater geosphere performance measures for ^{129}I and larger maximum ADEs from ^{129}I because of the increased rate of transport of ^{129}I through the rock of the geosphere.

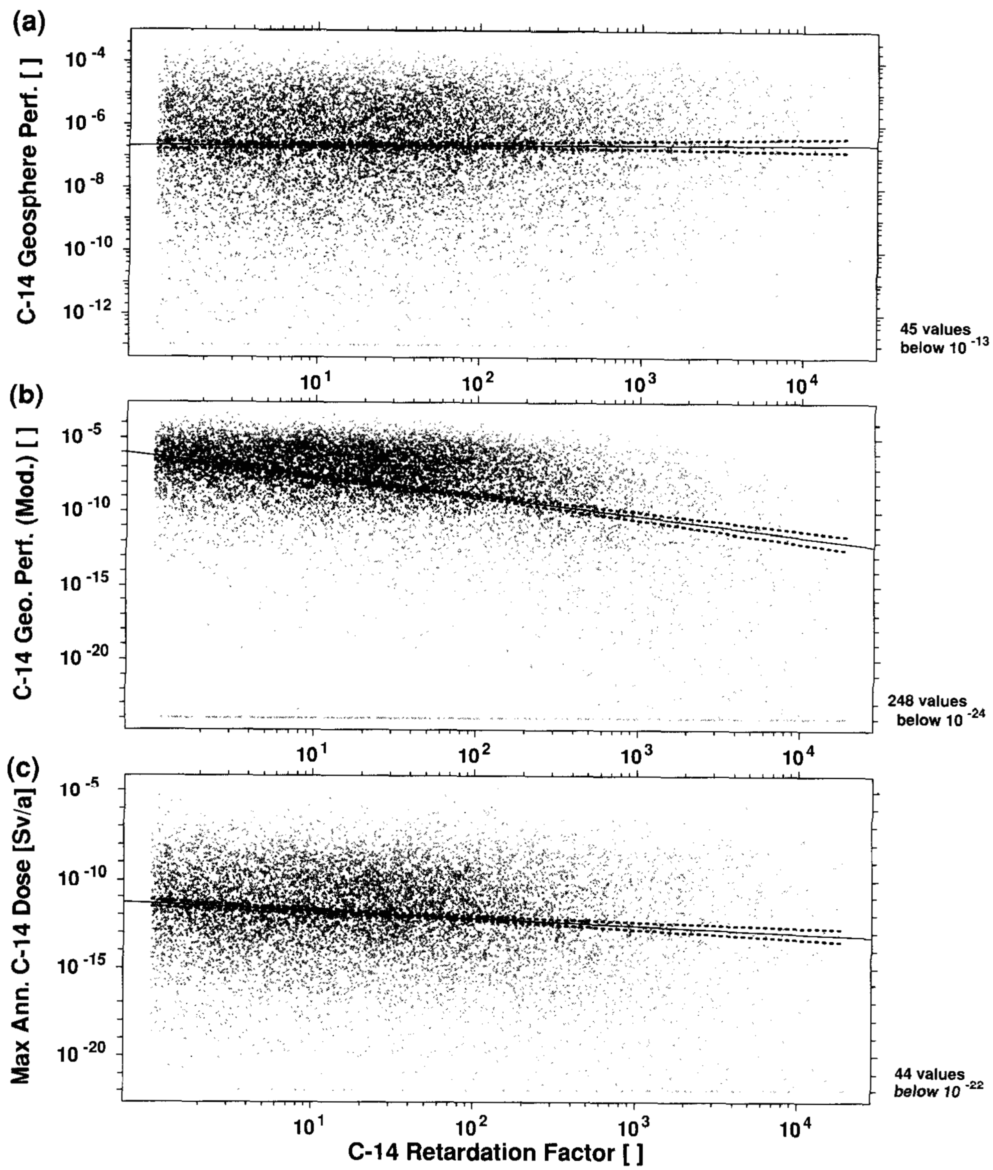


FIGURE E-20: Effect of Retardation Factor of Carbon in Compacted Organic Lake Sediment

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes plot the parameter describing the extent of sorption of ^{14}C on compacted organic lake sediment (expressed as a dimensionless retardation factor). The vertical axes are

(a) The (original) geosphere performance measure for ^{14}C over 10^5 a;
(b) A modified geosphere performance measure, defined to be the total estimated amount of ^{14}C that leaves the geosphere (where the exit point is taken to be the top of the compacted lake sediment) divided by the total amount of ^{14}C that enters the geosphere over 10^5 a; and
(c) The maximum ADE from ^{14}C up to 10^5 a.

The correlation coefficients for the trend lines are approximately 0.01 in part (a), -0.28 in part (b), and -0.15 in part (c). These plots show that larger retardation factors for carbon generally result in lower geosphere performance measures for ^{14}C and smaller maximum ADEs from ^{14}C because of additional delays in the transport of ^{14}C to the biosphere.

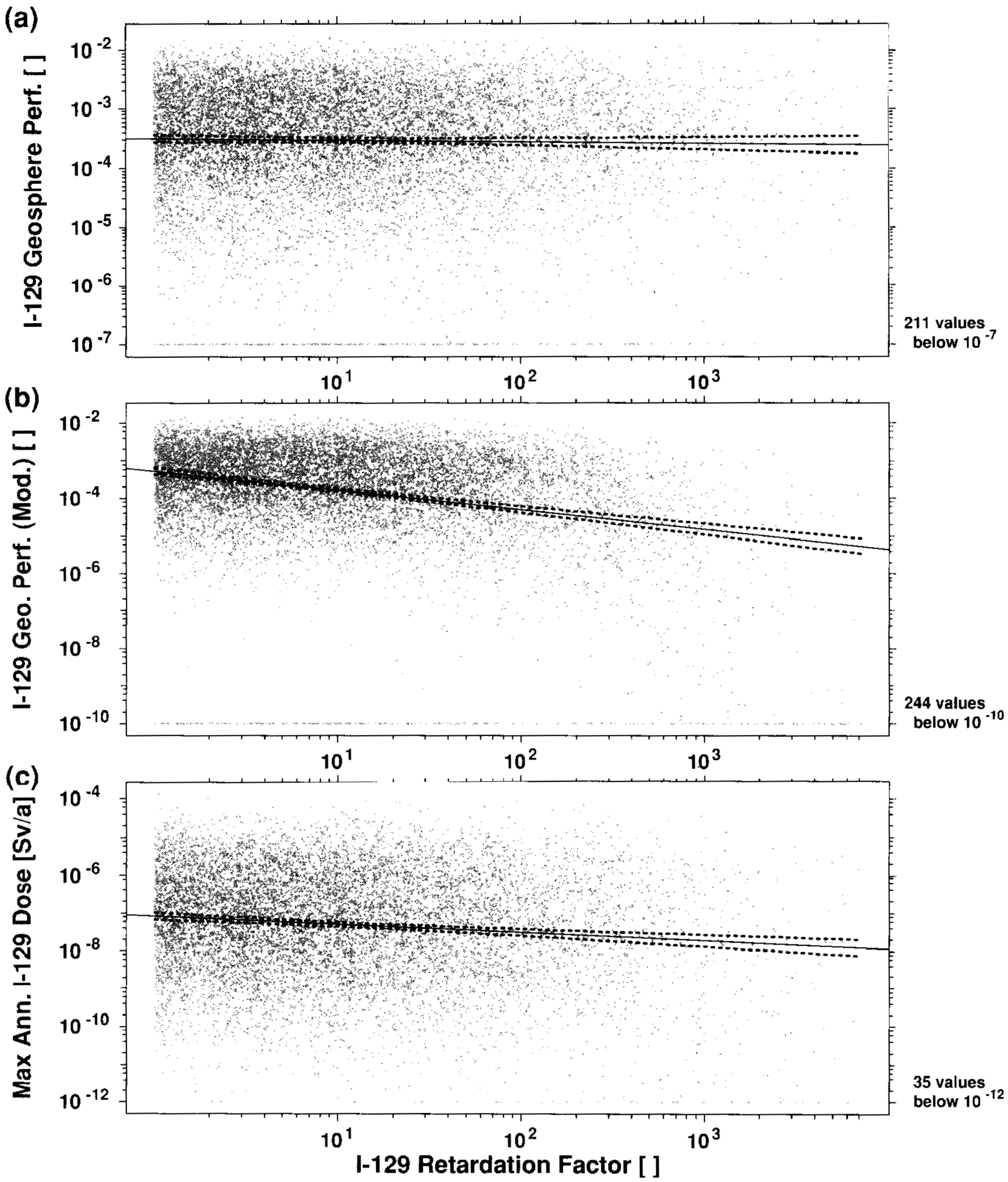


FIGURE E-21: Effect of the Retardation Factor of Iodine in Compacted Organic Lake Sediment

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes plot the parameter describing the extent of sorption of ^{129}I on compacted organic lake sediment (expressed as a dimensionless retardation factor). The vertical axes are

(a) The (original) geosphere performance measure for ^{129}I over 10^5 a;
(b) A modified geosphere performance measure, defined as the total estimated amount of ^{129}I that leaves the geosphere (where the exit point is taken to be the top of the compacted lake sediment) divided by the total amount of ^{129}I that enters the geosphere over 10^5 a; and
(c) The maximum ADE from ^{129}I up to 10^5 a.

The correlation coefficients for the trend lines are -0.01 in part (a), -0.20 in part (b), and -0.11 in part (c). These plots show that greater retardation factors for iodine generally result in smaller geosphere performance measures for ^{129}I and smaller maximum ADES from ^{129}I, because of additional delays in the transport of ^{129}I to the biosphere.

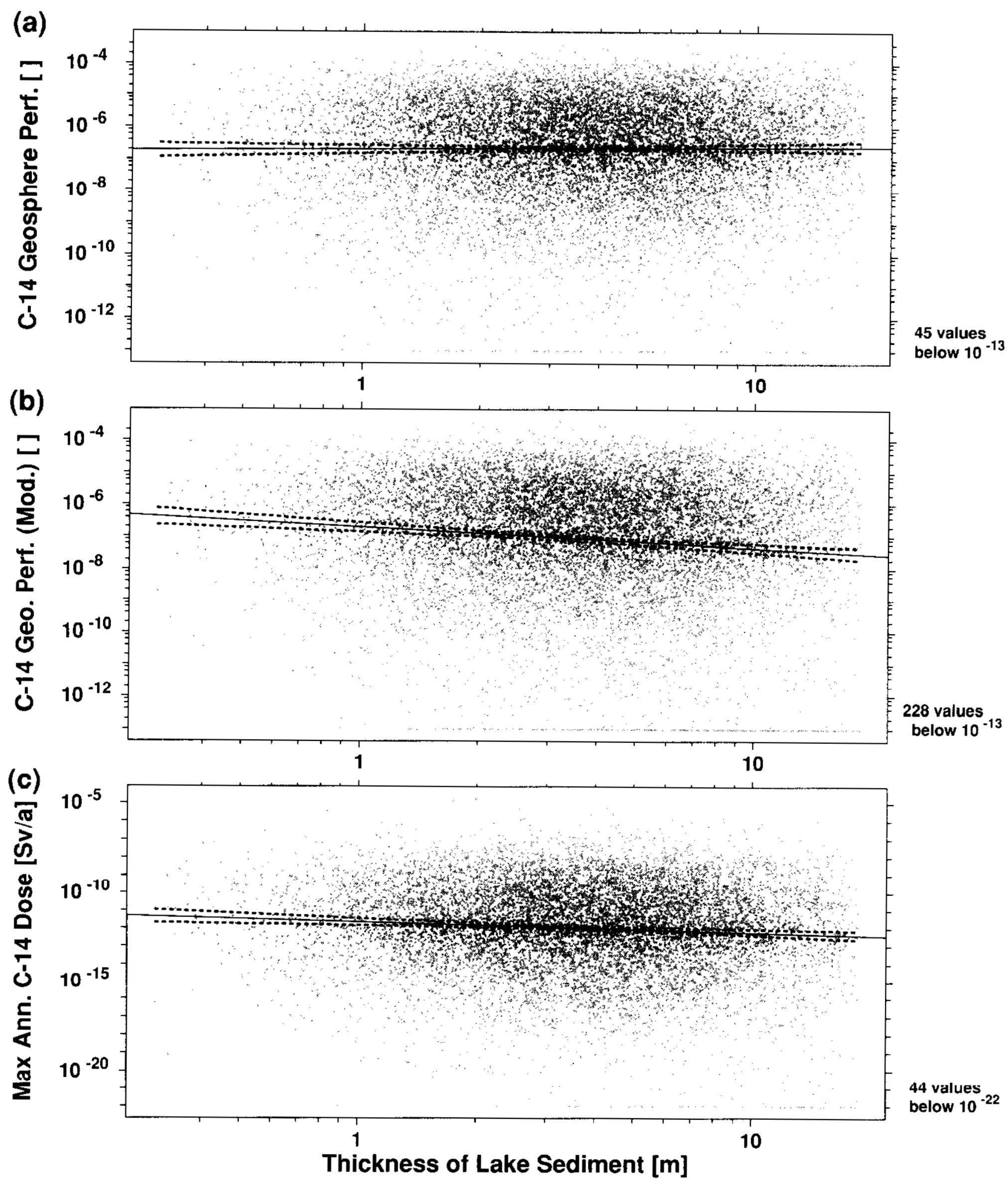


FIGURE E-22: Effect of the Thickness of Compacted Lake Sediment on Results for ^{14}C

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes plot the thickness of the compacted lake sediment at Boggy Creek South. The vertical axes are

(a) the (original) geosphere performance measure for ^{14}C over 10^5 a;
(b) a modified geosphere performance measure for ^{14}C (see text) over 10^5 a; and
(c) the maximum ADE from ^{14}C up to 10^5 a.

The correlation coefficients for the trend lines are 0.02 in part (a), -0.12 in part (b), and -0.07 in part (c). These plots show that greater thicknesses of the compacted organic lake sediment generally result in smaller geosphere performance measures for ^{14}C and maximum ADEs from ^{14}C because of additional delays in the transport of ^{14}C to the biosphere.

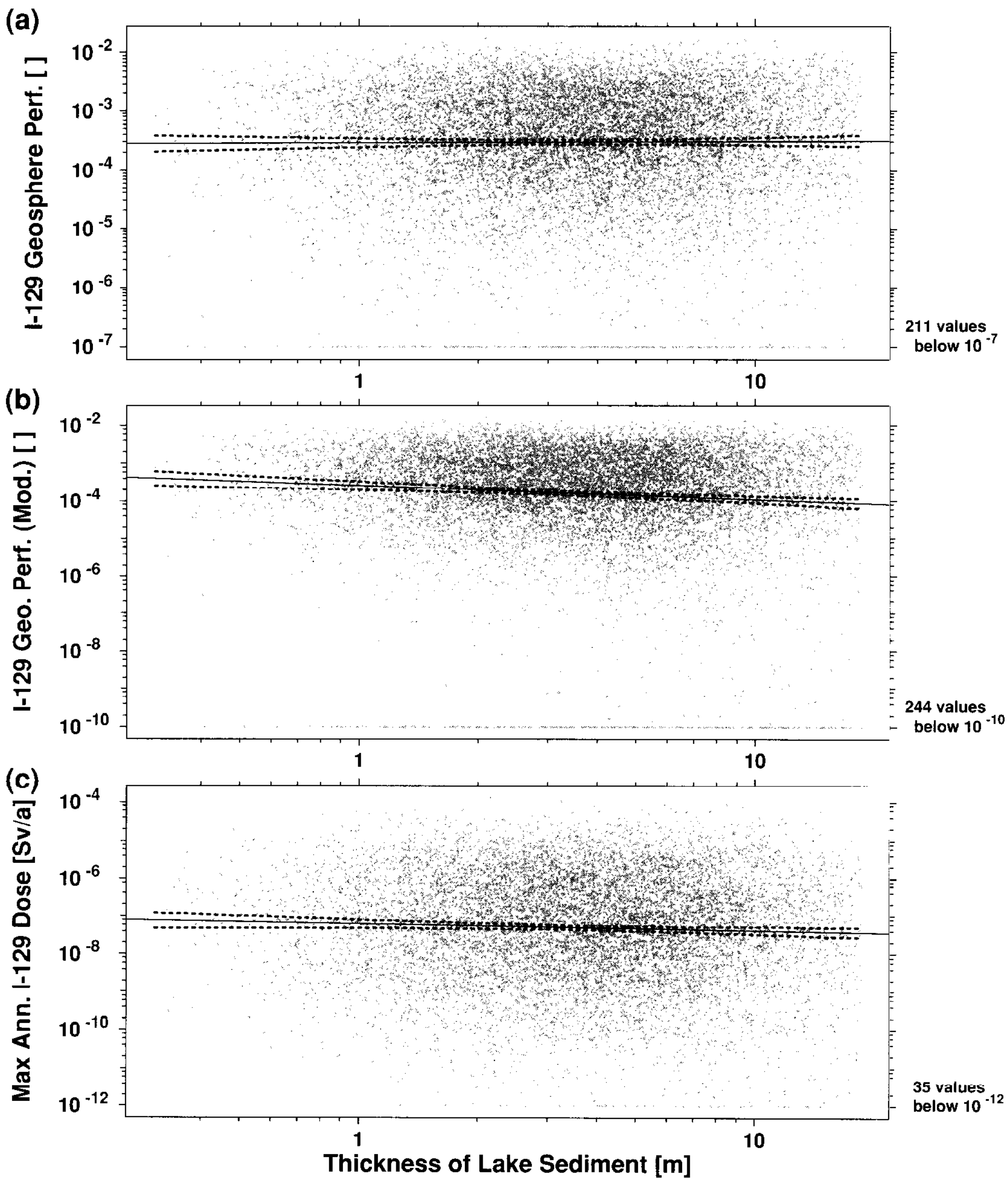


FIGURE E-23: Effect of the Thickness of Compacted Lake Sediment on Results for ^{129}I

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes plot the thickness of the compacted lake sediment at Boggy Creek South. The vertical axes are

(a) the (original) geosphere performance measure for ^{129}I over 10^5 a;
(b) a modified geosphere performance measure for ^{129}I (see text) over 10^5 a; and
(c) the maximum ADE from ^{129}I up to 10^5 a.

The correlation coefficients for the trend lines are 0.00 in part (a), -0.08 in part (b), and -0.04 in part (c). These plots show that greater thicknesses of the compacted organic lake sediment generally result in smaller geosphere performance measures for ^{129}I and maximum ADEs from ^{129}I because of additional delays in the transport of ^{129}I to the biosphere.

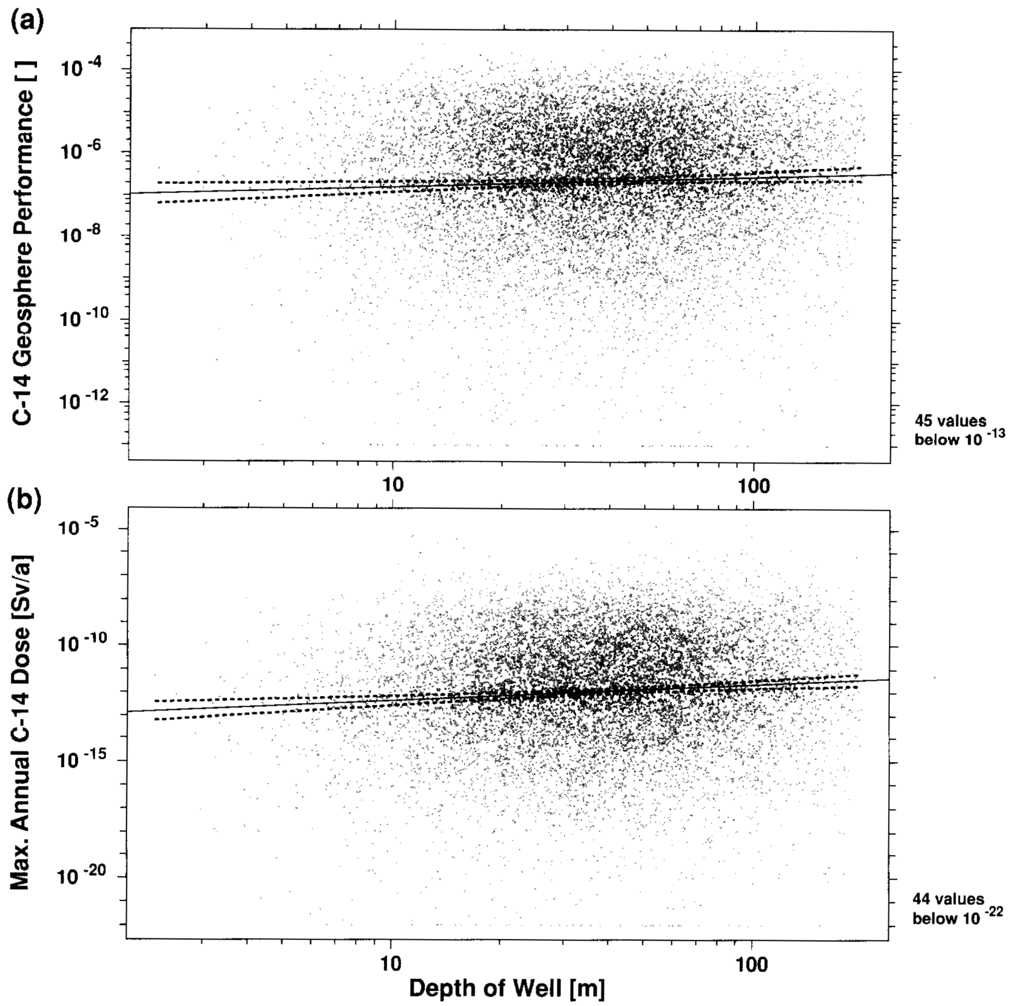


FIGURE E-24: Effect of the Well Depth on Results for ^{14}C

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes plot the depth of the well used to supply water to the critical group. The vertical axes are

(a) the (original) geosphere performance measure for ^{14}C over 10^5 a; and
(b) the maximum ADE resulting from ^{14}C up to 10^5 a.

The correlation coefficients for the trend lines are 0.03 in part (a) and 0.08 in part (b). These plots show that deeper wells tend to result in larger geosphere performance measures for ^{14}C and maximum ADEs from ^{14}C, although the effects are extremely weak.

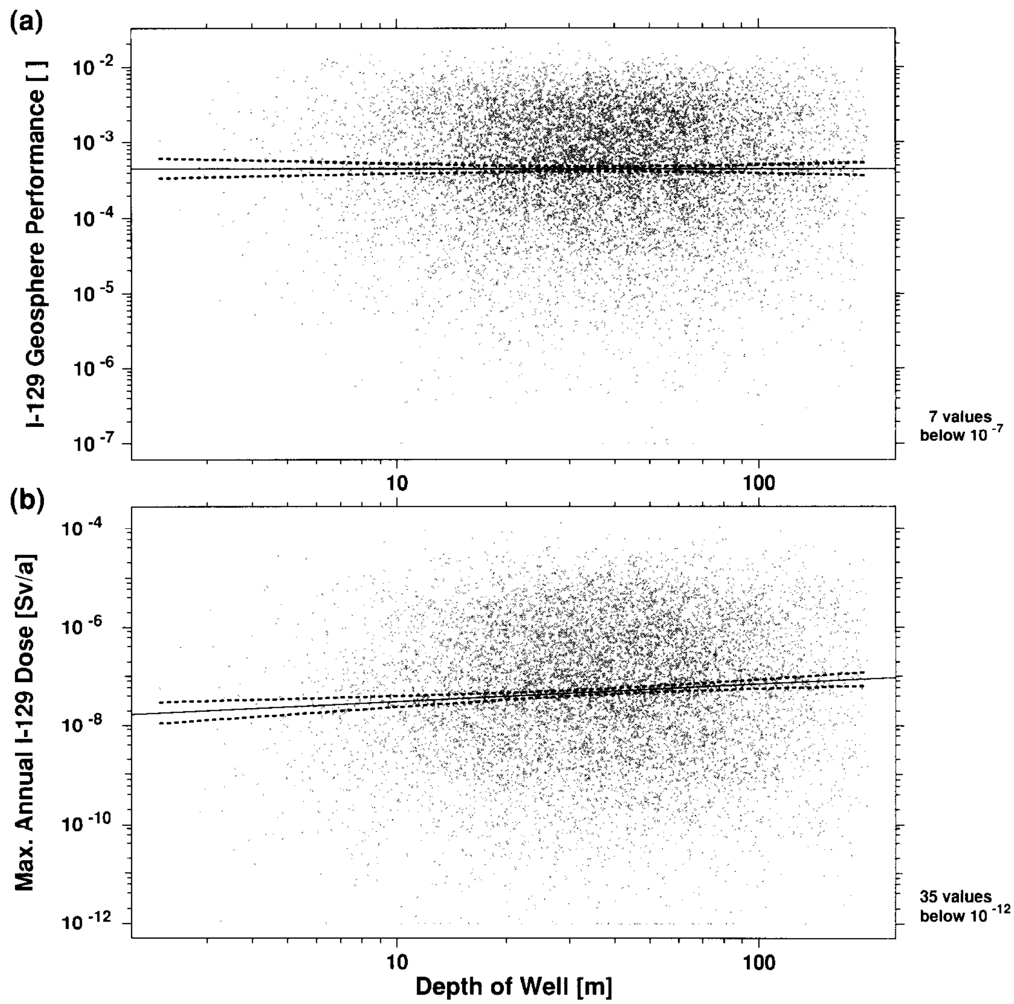


FIGURE E-25: Effect of the Well Depth on Results for ^{129}I

These scatter plots show the results from 10 000 randomly sampled simulations. The horizontal axes plot the depth of the well used to supply water to the critical group. The vertical axes are

(a) the (original) geosphere performance measure for ^{129}I over 10^5 a; and
(b) the maximum ADE from ^{129}I up to 10^5 a.

The correlation coefficients for the trend lines are -0.03 in part (a) and 0.06 in part (b). These plots show that deeper wells tend to result in larger maximum ADEs from ^{129}I (although the effects are very weak), and no obvious or very weak effects on the geosphere performance measure for ^{129}I.

Deeper wells correspond to shorter paths through the rock of the geosphere, and it might be expected that the slopes of the trend lines would be steeper (and positive). However, we note that bedrock wells are not deep enough to penetrate the lower rock zone of the geosphere, which is by far the most effective barrier in the geosphere model. Moreover, the sensitivity analysis for the median-value simulation shows that contaminant transport to the well is a complex function of many parameters, including the depth of the well, the groundwater velocity scaling factor and the number of persons making up the household of the critical group. The discussion in Section 6.3.3.3 of the main text, and in Section D.7.4 of Appendix D shows that the importance of the well is somewhat artificial when considering together both bedrock and overburden wells (because the use an overburden well for domestic water supply has effects similar to the use of the lake). Section 6.7.4 in the main text shows a weak effect remains when considering only bedrock wells; for example, Figure D-53 in Appendix D shows that the maximum ADE increases to a maximum near a well depth of 50 m, followed by a gradual decrease, resulting from the combined effects of plume capture and surface water dilution (Section D.7.4 in Appendix D). We expect similar complicating effects would occur in each of the randomly sampled simulations, but the effects are too small to be readily observed in Figures E-24 and E-25.

E.6 SENSITIVITY ANALYSIS OF THE BIOSPHERE MODEL

E.6.1 IMPORTANT PARAMETERS OF THE BIOSPHERE MODEL

The screening of parameters from the probabilistic simulations of the system model has identified one important parameter used in the biosphere model (Table 6-13 in the main text):

- The switch for source of domestic water, describing the choice between the use of lake water or well water as the source of domestic water used by the critical group.

This parameter is important in the probabilistic simulations in the sense that selecting one or other of the two options results in significant changes to the maximum ADEs.

Another fractional factorial screening study was directed at the biosphere performance measures for ^{129}I and ^{14}C. The biosphere performance measure for ^{129}I is defined as the ratio of two integrals evaluated for times up to 10^5 a: an interim integral of the ADE from ^{129}I is divided by the total amount of ^{129}I that enters the biosphere. This performance measure (with units of Sv/mol) provides an approximation of the total radiation dose attributed to the arrival of one mole of ^{129}I at the biosphere. A similar performance measure is defined for ^{14}C. For both radionuclides, the "interim" integral excludes isotopic dilution (which tends to obscure some effects). This study identified the above parameter and four additional parameters that have the largest effects on the two performance measures (Table E-1):

- the aquatic mass loading coefficient for iodine, describing the release of iodine from a surface water body by degassing;

- the gaseous evasion rate from soil for iodine, describing the loss of ^{129}I from soil by degassing;

- the plant/soil concentration ratio for iodine, giving contaminant concentrations in plants relative to concentrations in the soil on which they grow; and

- the gaseous evasion rate from soil for carbon describing the rate of ^{14}C from soil by degassing.

We also examine three additional parameters. The first is a switch affecting an option in the biosphere:

- the switch that selects use of lake sediment as soil in the garden, forage field, woodlot and peat bog (this parameter displays a weak effect in Table E-1).

The other two parameters are used to include the effects of isotopic dilution of ^{129}I and ^{14}C when estimating annual dose to members of the critical group. They are known to have significant effects; however, they were excluded from the biosphere performance measures so that the effects of other parameters could be observed. These two parameters are

- the concentration of stable iodine (as ^{127}I) found in typical groundwaters, and

- the concentration of stable isotopes of carbon (^{12}C and ^{13}C) found in typical groundwaters.

A number of other parameters listed in Table E-1 have relatively weak effects and are not discussed further. They include the ^{129}I plant environmental half-life (the time required for loss from the exposed plant parts of half the initial amount of deposited iodine, through biological processes and radioactive decay); the plant/soil concentration ratio for carbon; the size of the critical group; and the plant-to-mammalian meat coefficient for carbon.

All the parameters listed above are also identified in sensitivity analysis of the median-value simulation (Section 6.3.3 in the main text). In general, the effects of most of these parameters are much smaller for the probabilistic simulations than for the median-value simulation because of the obscuring influence of variations in all other parameters. However, all the parameters show the same trends in both the deterministic and probabilistic analyses.

In the following analysis, we group the eight parameters listed above into three categories:

- Water and land use parameters. This category includes the two switch parameters, describing the source of domestic water supply and the use of lake sediment as soil.

- Carbon and iodine ingestion parameters. This category includes the effect of the gaseous evasion rates from soil for iodine and carbon, the aquatic mass loading coefficient (from the lake) for iodine, and the plant/soil concentration ratio for iodine.

- Background Concentrations. The two parameters of interest here are the naturally occurring concentrations of stable isotopes of iodine and carbon in groundwater.

As in the two previous sections, scatter plots are used to show the effects of the important parameters. Each plot includes a trend line and its associated 95% confidence bands. The trend line (or regression line) is the least-squares fit (Section A.4.3.2 in Appendix A) to the logarithm of the parameter values and the logarithm of the estimated variables. The associated 95% confidence bands put bounds on the location of this trend line (Section A.4.3.3 in Appendix A).

Correlation coefficients measure the extent to which the data fits the regression line (Section A.4.3.2 in Appendix A). The degree of spread of data points about the trend line is a reflection of the effects of the range of possible values of the other parameters. Correlation coefficients vary from +1 to -1: values near +1 or -1 indicate a linear relationship between the estimated variable and the parameter, whereas values near zero implies no such relationship exists.

One difference exists for the plots of the two switch parameters. For most scatter plots, the horizontal axis shows the parameter of interest, with values that fall anywhere within the range of permitted values. However, the switch parameters only take on several discrete values, and these values cannot be used to produce a meaningful scatter plot. Thus we use different types of plots for the switch parameters.

E.6.2 EFFECTS OF WATER AND LAND-USE PARAMETERS

The two switch parameters included in this group select whether the source of domestic water is a well or the lake and whether fresh lake sediment is used as soil.

Figures E-26 and E-27 show the effect of the switch selecting well water or lake water for domestic needs, for estimated doses from ^{14}C and ^{129}I respectively. Comparison of the trend lines shows that dose estimates tend to be greater if the critical group uses the well instead of the lake for their water supply. This is true for the majority but not all the different combinations of parameter values. The presence or absence of the well is less important in sensitivity analysis of the probabilistic simulations than in the median-value simulation (Section D.8.2 in Appendix D) because the variation in dose estimates caused by changes in the other parameters obscures the effect of even this very influential switch. Further examination of the statistics for the data in these figures shows that ADEs from the use of well water tend to be larger for smaller sizes of the critical group.

The results in Table E-1 show that the mean ADE is weakly affected by the switch selecting fresh lake sediment as soil. The PDF for this switch is defined such that sediment is farmed in only 1% of simulations for the reference disposal system. To ensure that we have a converged estimate of its effects, we performed an extra 1000 simulations but modified the switch data so that the sediment option was always selected. Figure E-28 displays the results. The figure show the mean ADEs from ^{14}C and ^{129}I when sediment

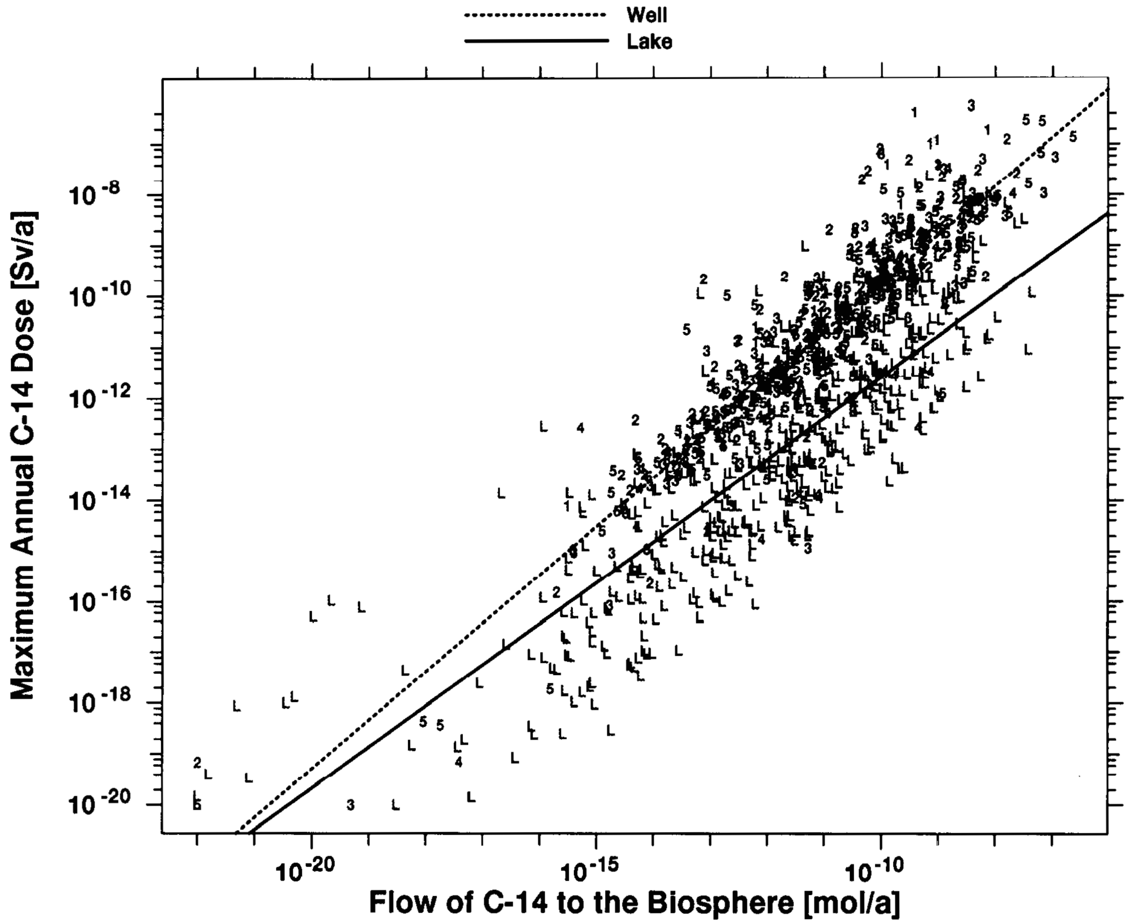


FIGURE E-26: Effect of the Switch Selecting Source of Water on Annual Dose Estimate from ^{14}C

This scatter plot shows the effect of the switch that selects the well or the lake as the source of domestic water used by the critical group. The vertical axis is the maximum, up to 10^5 a, of the ADE from ^{14}C. The horizontal axis is the estimated maximum, up to 10^5 a, of the flow of ^{14}C into the sediment and the well. Results are shown for 1000 randomly sampled simulations (about 500 each for the well and for the lake); each symbol plots the result of one simulation:

- "L" identifies simulations involving the use of the lake; and
- "1" to "4" and "5" identify simulations involving the use of the well by a critical group consisting of 1 to 4 and 5 or more individuals.

The two trend lines are computed from least squares fitting to the logarithms of the data for the lake and the data for the well. The correlation coefficients are 0.87 for the simulations involving the well and 0.90 for the simulations involving the lake. The results show that dose estimates tend to be larger when the well is the source of domestic water and larger for a smaller sized critical group.

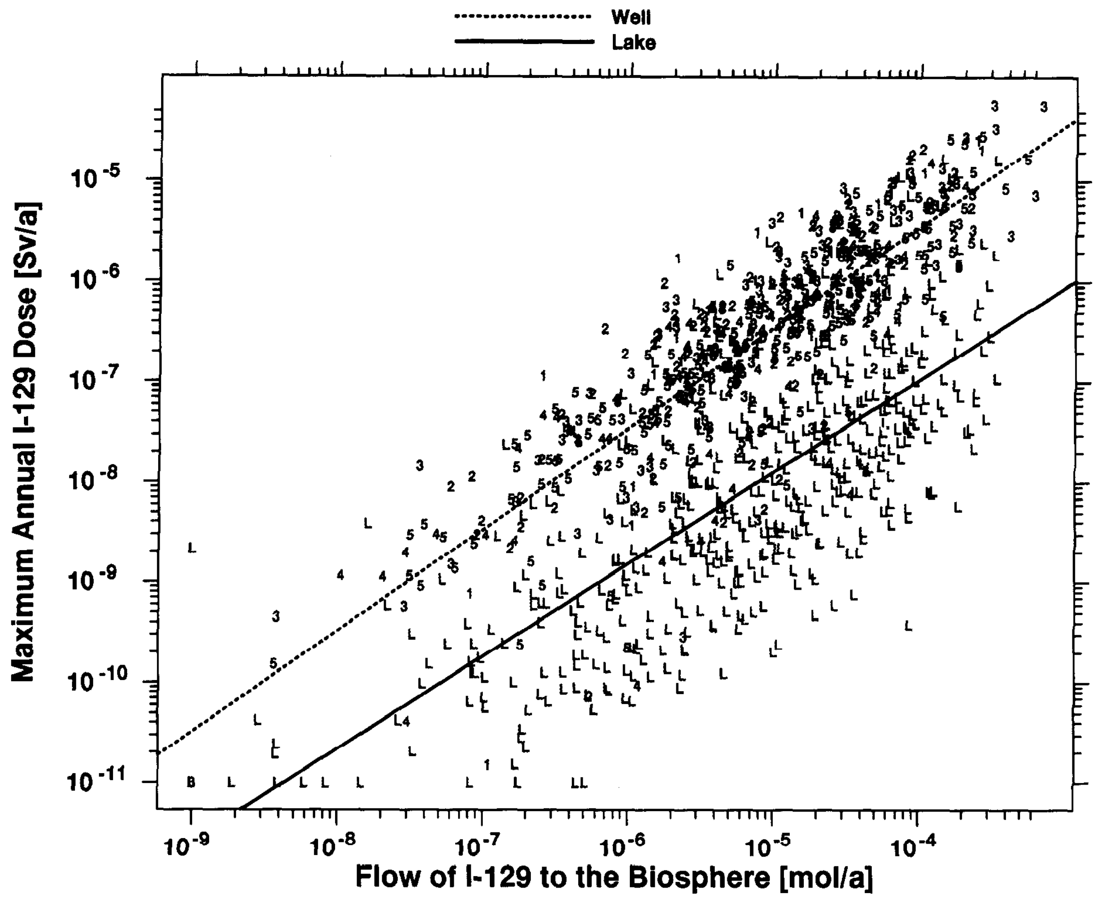


FIGURE E-27: Effect of the Switch Selecting Source of Water on Annual Dose Estimate from ^{129}I

This scatter plot shows the effect of the switch that selects the well or the lake as the source of domestic water used by the critical group. The vertical axis is the maximum, up to 10^5 a, of the ADE from ^{129}I. The horizontal axis is the estimated maximum, up to 10^5 a, of the flow of ^{129}I into the sediment and the well. Results are shown for 1000 randomly sampled simulations (about 500 each for the well and for the lake); each symbol plots the result of one simulation:

- "L" identifies simulations involving the use of the lake, and
- "1" to "4" and "5" identify simulations involving the use of the well by a critical group consisting of 1 to 4 and 5 or more individuals.

The correlation coefficients for the trend lines are 0.85 for the simulations involving the well and 0.61 for the simulations involving the lake. The results show that dose estimates tend to be larger when the well is the source of domestic water and larger for a smaller sized critical group.

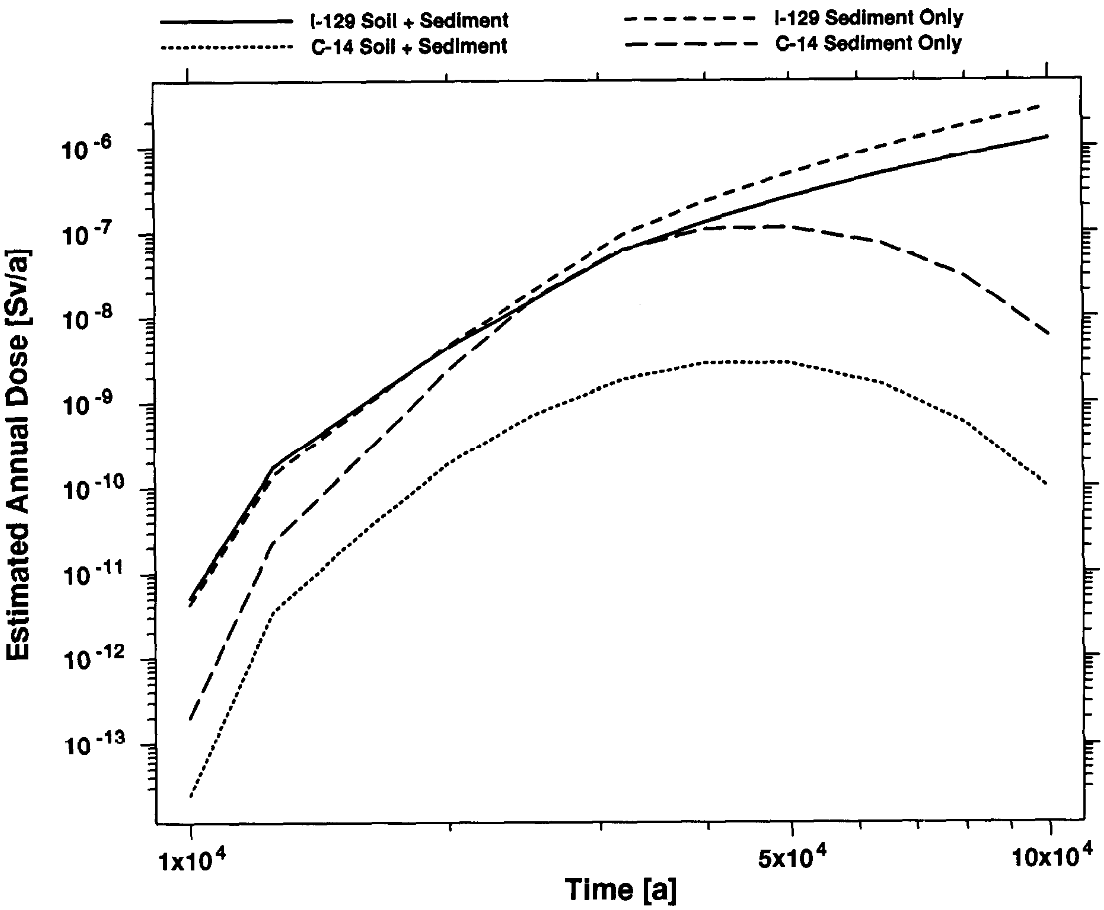


FIGURE E-28: Effect of the Switch Selecting the Use of Lake Sediment as Soil

This figure shows the results from two sets of 1000 simulations:

- For the curves labelled "Soil + sediment", the simulations are the first 1000 used in the probabilistic analysis (Section 6.5.2) and correspond to a case where lake sediment is used as soil in about 1% of the simulations (or 10 of the 1000 simulations); and
- For the curves labelled "Sediment only", we have modified the PDF for the switch so that lake sediment is used as soil in all of the 1000 simulations (all other parameters are assigned the same sequence of randomly selected values as in the "Soil + sediment" simulations).

The four curves show the arithmetic means of the ADEs from ^{14}C and from ^{129}I as a function of time. The use of lake sediment as soil leads to greater mean annual doses for both ^{129}I and ^{14}C because we assume these volatile contaminants degass from soil but not fresh lake sediment. The effects are more pronounced for ^{14}C because its gaseous evasion rate is about 200 times greater than the gaseous evasion rate for ^{129}I (see text).

is used as soil as originally defined (in about 1% of the simulations) and when sediment is used as soil in all simulations.

Use of lake sediment as soil tends to increase the ADEs, with greater effects on doses from ^{14}C than from ^{129}I. The effect is most noticeable for ^{14}C because of the effect of degassing. In the biosphere model, we assume that volatile contaminants (which include ^{129}I and ^{14}C) are lost from terrestrial soil through degassing. However, we also assume that no degassing occurs when lake sediment is used as soil. This results in higher concentrations of volatile contaminants in lake sediment used as soil, higher concentrations of ^{129}I and ^{14}C in the plants consumed by the critical group, and hence larger ADEs. The effects are much more pronounced for ^{14}C because its gaseous evasion rate from soil is about 200 times greater than the gaseous evasion rate of ^{129}I from soil (see Section D.8.2 in Appendix D).

E.6.3 EFFECTS OF IODINE AND CARBON INGESTION PARAMETERS

The four parameters included in this group are

- the aquatic mass loading coefficient (from the lake) for iodine,
- the gaseous evasion rate from soil for iodine,
- the plant/soil concentration ratio for iodine, and
- the carbon gaseous evasion rate from soil.

Figure E-29 shows the effect of the aquatic mass loading coefficient for iodine on the maximum estimated dose from ^{129}I, up to 10^5 a. Greater values of this parameter correspond to more degassing of ^{129}I from the lake. Part (a) shows results from 10 000 randomly selected simulations. Parts (b) and (c) of the figure both use the same data but show separately the results for simulations involving the well and the lake. The trend lines show that the estimated doses tend to increase for increased values of the aquatic mass loading coefficient. This is the expected result because greater values of the coefficient correspond to greater concentrations of ^{129}I in the air and to greater contamination of the plants consumed by members of the critical group. The slope of the trend line is largest in part (c), which shows results from simulations where no well is present. The slope is smaller in parts (a) and (b) because of the greater importance of pathways involving the use of well water relative to pathways involving air deposition from contaminants in the lake.

Figure E-30 shows the effect of the gaseous evasion rate from soil for iodine on the maximum estimated dose from ^{129}I, up to 10^5 a. Greater values of this parameter correspond to more degassing of ^{129}I from the soil and, therefore, lower concentrations of ^{129}I in soil but greater concentrations in air. In turn, there would be lower concentrations in the plants consumed by the critical group (because air deposition is less significant than root uptake). Thus the slope of the trend line is negative, although the correlation coefficient shows that the overall effect of this parameter is relatively weak. (Recent experimental data, discussed further in

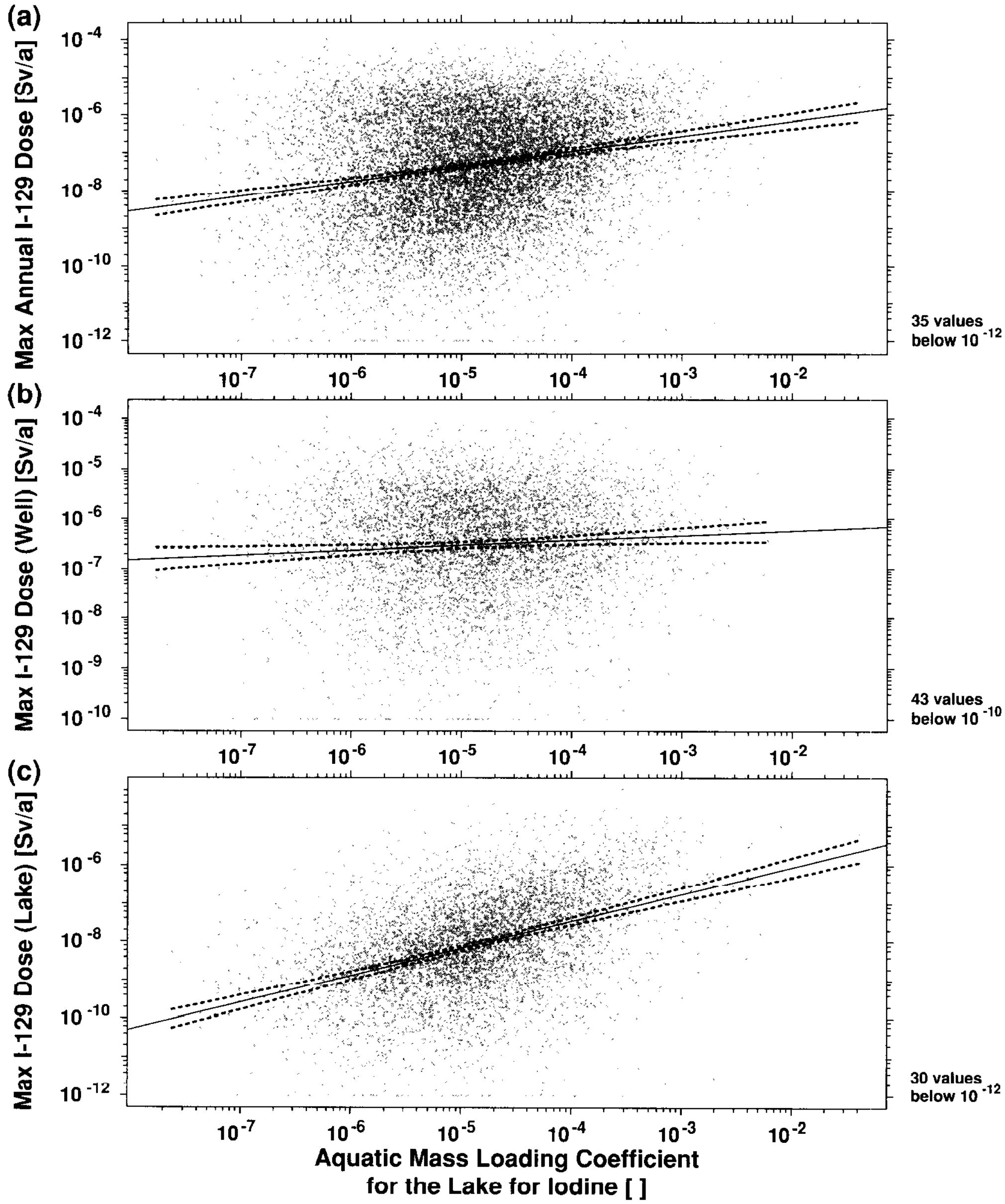


FIGURE E-29: Effect of the Aquatic Mass Loading Coefficient for Iodine

This scatter plot shows the effect of the (dimensionless) parameter that describes the release of ^{129}I from lake water to the air by degassing. Once in the air, ^{129}I may contaminate plants by deposition. The horizontal axis is the aquatic mass loading coefficient for iodine. The vertical axis is the maximum, up to 10^5 a, of the estimated annual dose from ^{129}I. Results are shown for 10 000 randomly sampled simulations; each symbol plots the result of one simulation:

(a) shows the results from all 10 000 simulations,
(b) shows the results from about 5000 simulations where the source of domestic water is the well, and
(c) shows the results from the other (approximately 5000) simulations where the source of domestic water is the lake.

The correlation coefficients for the trend lines are 0.22 for part (a), 0.07 for part (b), and 0.42 for part (c). The slopes of the trend lines are positive (as expected), indicating that a greater release of iodine from the lake leads to a greater contamination of plants consumed by members of the critical group. Parts (a) and (b) show smaller effects than part (c) because of the relative importance of pathways other than air deposition.

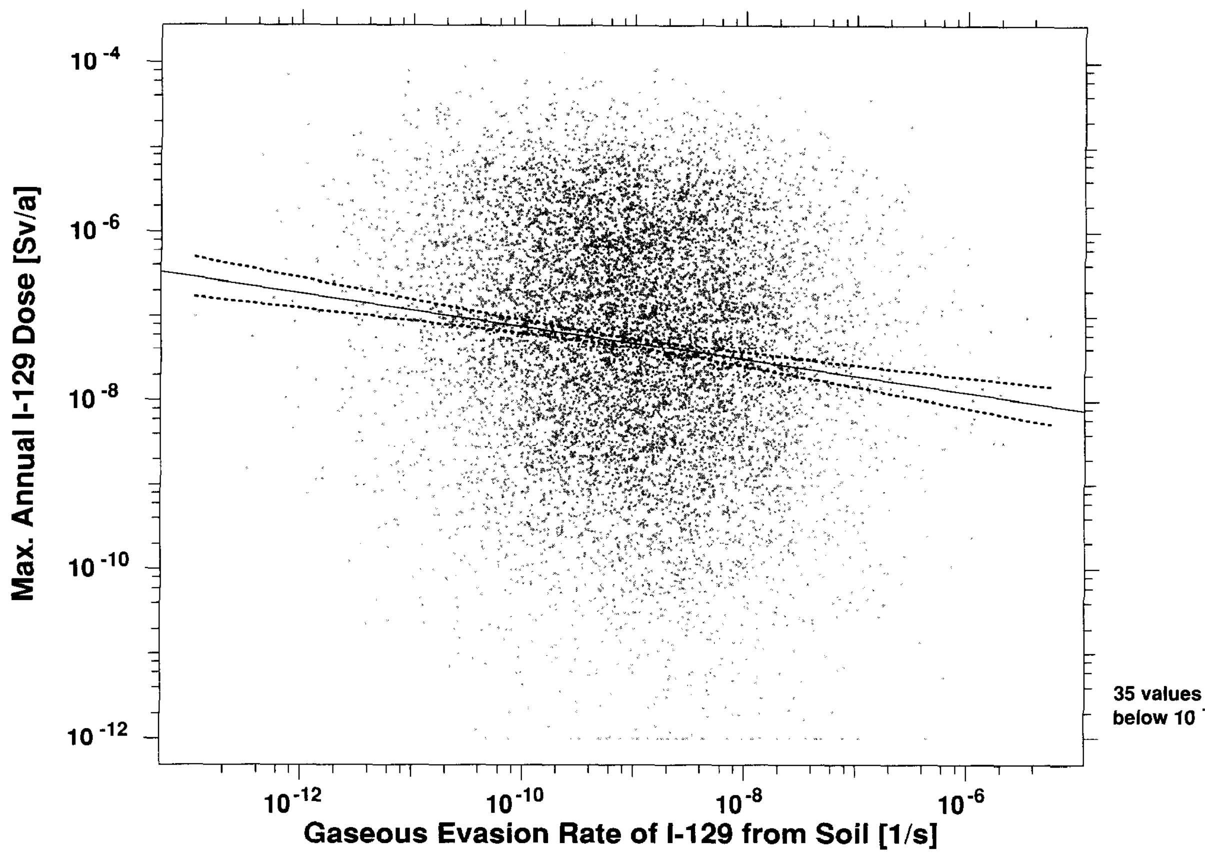


FIGURE E-30: Effect of the Gaseous Evasion Rate from Soil for Iodine

This scatter plot shows the effect of the parameter that describes the release rate of ^{129}I from soil to the air by degassing. The horizontal axis is the gaseous evasion rate from the soil for iodine. The vertical axis is the maximum, up to 10^5 a, of the estimated annual dose from ^{129}I. Results are shown for 10 000 randomly sampled simulations; each symbol plots the result of one simulation.
The correlation coefficient for the trend line is -0.13. The slope of the trend line is negative (as expected) because greater gaseous evasion rates correspond to lower concentrations of ^{129}I in soil and in the plants consumed by members of the critical group.

Section 8.2.6 in the main text, suggest that a smaller gaseous evasion rate from soil should be used for iodine, which would lead to slightly greater estimates of annual dose from ^{129}I.)

Figure E-31 shows the effect of the plant/soil concentration ratio on the maximum ADEs from ^{129}I. The trend line shows a weak tendency for increased doses with increased values of the concentration ratio. More pronounced effects may be observed through the judicious use of intermediate variables; for example, results not shown here indicate stronger trends using an interim estimate of dose that considers only ingestion of garden produce and that excludes the effects of isotopic dilution. This is the expected result because greater ratios correspond to higher concentrations of ^{129}I in plants consumed by the critical group and, therefore, larger estimates of annual dose.

Figure E-32 shows the effect of the carbon gaseous evasion rate from soil on the maximum ADEs from ^{14}C. Estimated doses from ^{14}C are consistently smaller than estimated doses from ^{129}I and, therefore, this parameter does not have important effects on the total ADEs. The figure shows that doses from ^{14}C tend to decrease as the carbon gaseous evasion rate increases. This occurs, as discussed in Section D.8.3, because degassing reduces concentrations of ^{14}C in soil, which leads to smaller concentrations of ^{14}C in plants consumed by the critical group and, therefore, smaller doses from ^{14}C. The trend is weak, as evidenced by the relatively small value of the correlation coefficient. (Recent experimental data, discussed further in Section 8.2.6 in the main text suggest that a greater gaseous evasion rate from soil should be used for carbon, which would lead to smaller estimates of annual dose from ^{14}C.)

E.6.4 EFFECTS OF THE GROUNDWATER DILUTION LIMIT

Section 5.6 in the main text notes that ^{129}I and ^{14}C from the vault would be mixed and diluted with nonradioactive isotopes of iodine and carbon naturally present in groundwater. We include these effects in the biosphere model by imposing corresponding limits on possible internal doses from ^{129}I and ^{14}C, taking into account the dilution produced by their naturally occurring stable isotopes.

Figures E-33 shows the effect of the groundwater dilution limit for ^{129}I. The vertical axis plots the interim estimate of the annual dose; it is the ADE calculated without accounting for the dilution limit. The horizontal axis plots the final ADE, which includes adjustments for the groundwater dilution limit. Adjustments are required in 786 of the 1000 simulations but are generally relatively small. In about 15 simulations, the adjustment is greater than a factor of 100 because the limit allowed by the presence of stable iodine in groundwater is as much as 200 times smaller than the uncorrected estimate of internal dose from ^{129}I.

An adjustment is required much more frequently for simulations in which a well is present and, more frequently, for the simulations giving larger ADEs. This occurs because the well tends to be a more concentrated source of ^{129}I than the lake, and hence the well more frequently yields greater estimates of dose that are more likely to exceed the dilution limit.

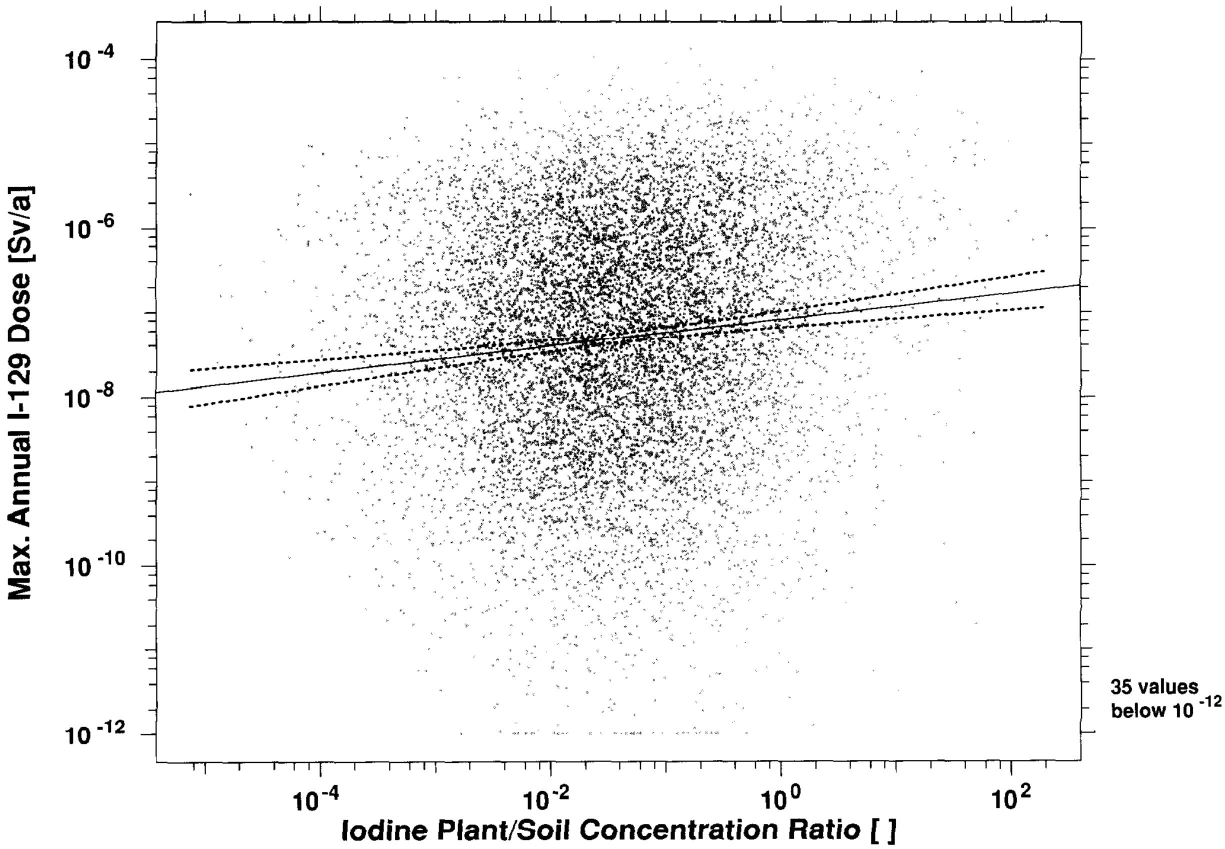


FIGURE E-31: Effect of the Plant/Soil Concentration Ratio for Iodine

This scatter plot shows the effect of the parameter that describes the transfer of ^{129}I from soils to plants, including plants grown in the garden used by the critical group. (The units of this parameter are shown as dimensionless; more accurately, they are (Bq/kg wet biomass)/(Bq/kg dry soil).) The horizontal axis is the iodine soil/plant concentration ratio. The vertical axis is the maximum, up to 10^5 a, of the estimated annual dose from ^{129}I. Results are shown for 10 000 randomly sampled simulations; each symbol plots the result of one simulation.
The correlation coefficient for the trend line is 0.10.

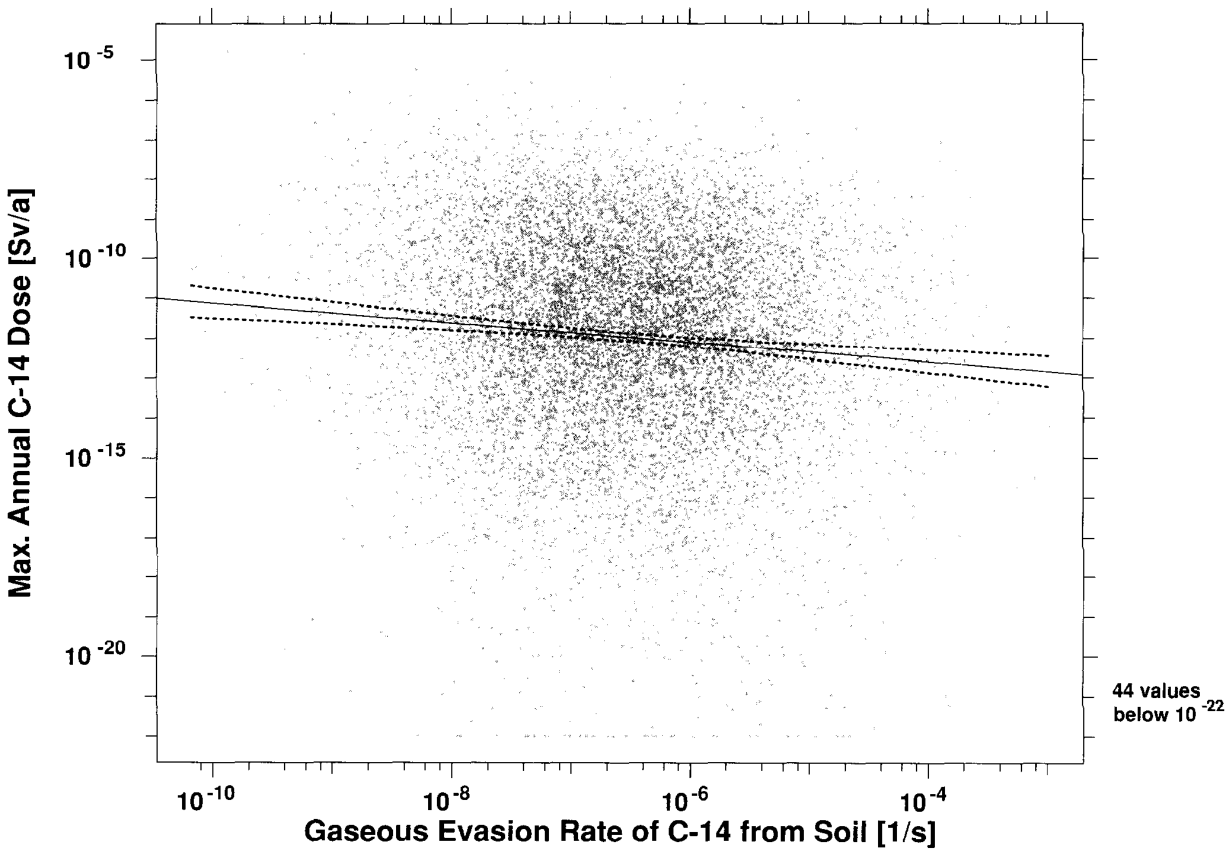


FIGURE E-32: Effect of the Carbon Gaseous Evasion Rate from Soil

This scatter plot shows the effect of the parameter that describes the release rate of ^{14}C from soil by degassing. The horizontal axis is the gaseous evasion rate of carbon from soil. The vertical axis is the maximum, up to 10^5 a, of the estimated annual dose from ^{14}C. Results are shown for 10 000 randomly sampled simulations; each symbol plots the result of one simulation.
The correlation coefficient for the trend line is -0.09. The slope of the trend line is negative (as expected) because greater gaseous evasion rates correspond to lower concentrations of ^{14}C in soil and in the plants consumed by members of the critical group. The effect of this parameter on annual dose estimate totalled over all radionuclides is relatively small because ^{129}I (and not ^{14}C) is the major contributor to the total ADE.

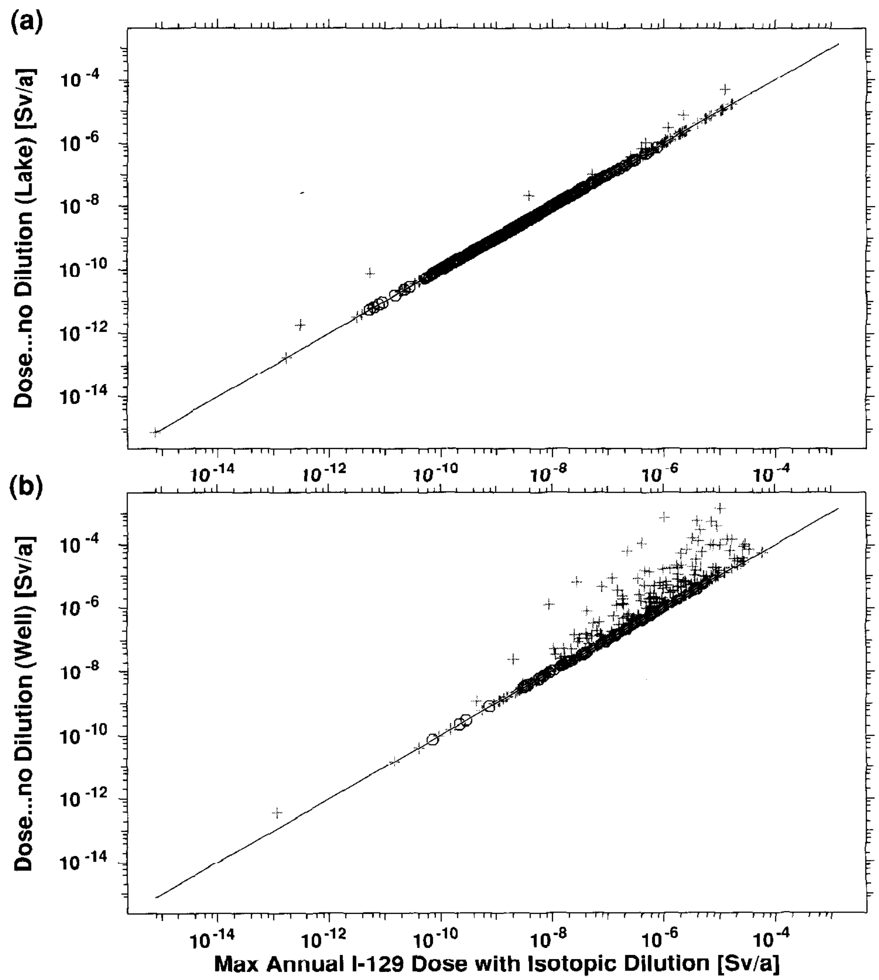


FIGURE E-33: Dose Adjustments Resulting from Isotopic Dilution by Stable Iodine

These figures show the effects of isotopic dilution on the maximum estimated annual doses from ^{129}I up to 10^5 a. The two figures are based on results from 1000 simulations; parts (a) and (b) respectively show results from simulations in which only the lake and only the well provide domestic water used by members of the critical group.
The vertical axis plots the ADE calculated without accounting for the dilution limit, and the horizontal axis plots the ADE with a correction for the groundwater dilution limit. The symbols identify individual simulations. The circles (on the diagonal line) indicate simulations where a correction resulting from the groundwater dilution limit is not used. The plus signs (above the diagonal) indicate, on the vertical axis, the magnitude of the annual dose without accounting for isotopic dilution. The corrected value would appear immediately below on the diagonal line.

Adjustments resulting from isotopic dilution are generally small and are more frequently required for simulations involving the well because the well tends to be a more concentrated source of ^{129}I than the lake.

Annual dose estimates from ^{14}C are also affected by isotopic dilution (Figure E-34), except that the groundwater dilution limit is rarely exceeded, and the subsequent dose reductions are relatively small.

E.7 ANALYSIS OF THE TORTUOSITY OF THE LOWER ROCK ZONE

E.7.1 INTRODUCTION

There is strong evidence that we have identified all the important parameters with respect to the maximum ADEs from the system model. These parameters are relatively few in number (eight in all; Table 6-13 in the main text) compared with the several thousand parameters appearing in the system model. Their effects on the maximum ADE in the probabilistic simulations ranges from strong in the case of the tortuosity of the lower rock zone to weak in the case of the depth of the well.

We examine in more detail in this section the effects of the tortuosity of the lower rock zone, one of the more important parameters from the sensitivity analyses (Sections 6.5.5 in the main text and E.3 to E.5). Its PDF for the reference disposal system represents a wide range of possible values and is based on studies of rock from the Canadian Shield, including rock from the WRA (Davison et al. 1994).

Tortuosity is a reducible parameter; that is, further experimental and field studies could reduce our uncertainties about its actual value. (We expect that some residual uncertainty would always remain if the tortuosity varies from place to place in the lower rock zone or if experimental measurements are imprecise.) Our analysis examines how worthwhile the effort could be. This and similar studies would be of value in providing guidance for further research efforts in support of a postclosure assessment. Related studies could also provide guidance for site characterization and site selection.

Tortuosity, a measure of the increase in transport distance across some geological media because of the winding nature of the interconnected aqueous pathway, affects only the diffusive part of the transport of contaminants (Davison et al. 1994). It is an empirically determined parameter that is dependent on other characteristics of the lower rock zone, such as permeability, porosity, and the types and amounts of minerals present. The PDFs for these parameters are chosen to be consistent with field and laboratory studies of the WRA (Davison et al. 1994). If a different PDF were chosen for tortuosity, then different PDFs may be required for other parameters for consistency.

As in preceding sections on probabilistic sensitivity analysis, we focus on the maximum ADEs to 10^5 a that result from ^{129}I and ^{14}C. Specifically, we examine the effects of changing the PDF for tortuosity of the lower rock zone on

- the maximum ADE from different simulations,
- the magnitude of the mean of the maximum ADEs from different sets of simulations, and

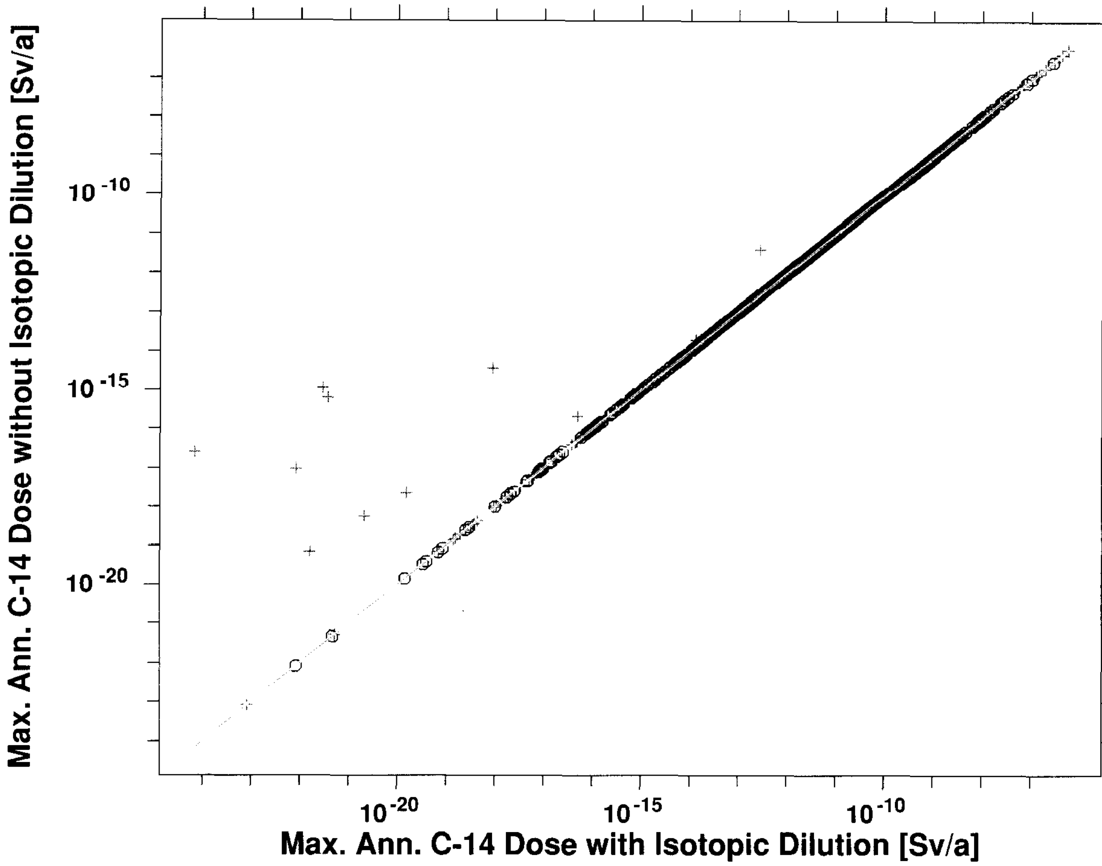


FIGURE E-34: Dose Adjustments Resulting from Isotopic Dilution by Stable Carbon

These figures show the effects of isotopic dilution on the maximum estimated annual doses from ^{14}C up to 10^5 a. The figure is based on results from 2000 simulations in which either the lake or the well provide domestic water used by members of the critical group.
The vertical axis plots the ADE calculated without accounting for the dilution limit, and the horizontal axis plots the ADE with a correction for the groundwater dilution limit. The symbols identify individual simulations. The circles (on the diagonal line) indicate simulations where a correction resulting from the groundwater dilution limit is not used. The plus signs (above the diagonal) indicate, on the vertical axis, the magnitude of the annual dose without accounting for isotopic dilution. The corrected value would appear immediately below on the diagonal line.

There are far fewer simulations where adjustments for isotopic dilution are required for ^{14}C compared with ^{129}I (Figure E-33).

- the spread or uncertainty in the mean of the maximum ADEs.

The mean of the maximum ADEs is the arithmetic average of the maxima in the ADEs. They are taken to 10^5 a from sets of 500 simulations and include the effects of uncertainty. (Note that the average of the maxima is an upper bound of the maximum of the averages because the maxima will occur a different times.)

For the reference disposal system, the specified PDF for the tortuosity of the lower rock zone is triangular with a range from 2 to 8 and with a most probable value (the mode) equal to 3 (Davison et al. 1994). This function is shown as PDF A in Figure E-35. The other PDFs in this figure are variants of PDF A, discussed in the analysis below. Table E-6 lists the values of the attributes corresponding to PDFs A through E of Figure E-35. As indicated in the figure and in the table

- PDF A and PDF B have the same mean but differing widths,

- PDF B and PDF D have the same width but different means, and

- PDF C and PDF D have approximately the same mode but different widths.

- PDF E has a larger lower bound, mode and mean than the other PDFs.

The set of PDFs was chosen to keep all parameter values within the original range and to preserve the triangular shape of the original PDF. Similar studies could be carried out for other ranges and for other types of PDFs.

Part of the analysis uses five sets of 500 simulations, each involving one of these five PDFs. In each set of simulations, we use the same sequence of randomly sampled values for all parameters, except for the tortuosity of the lower rock zone. Values for the tortuosity differ because this parameter is described using different PDFs. However, the sampling of tortuosity is such that the sampled values have the same sequence of quantiles.

That is, for a simulation in which an extreme value is selected from PDF A, then a corresponding extreme value would be selected from PDF E; if a central value is selected from PDF A, then a corresponding central value would be selected from PDF E. This sampling scheme ensures that the same "mix" of sampled values are used, and it maximizes the information obtained from the comparisons.

E.7.2 EFFECTS OF CHANGING THE MEAN VALUE OF THE PDF

Probability density functions B and D have the same width and shape, but their ranges and modes differ. The sampling scheme in the 500 random simulations is such that all values of the tortuosity are larger by 1.17 (additive) when using PDF B, compared with PDF D. That is, if a sampled value using PDF D is equal to 3.00, then the value using PDF B would be 4.17, and thus the mean of the tortuosity is larger by about 1.17, or 36%, when using PDF B.

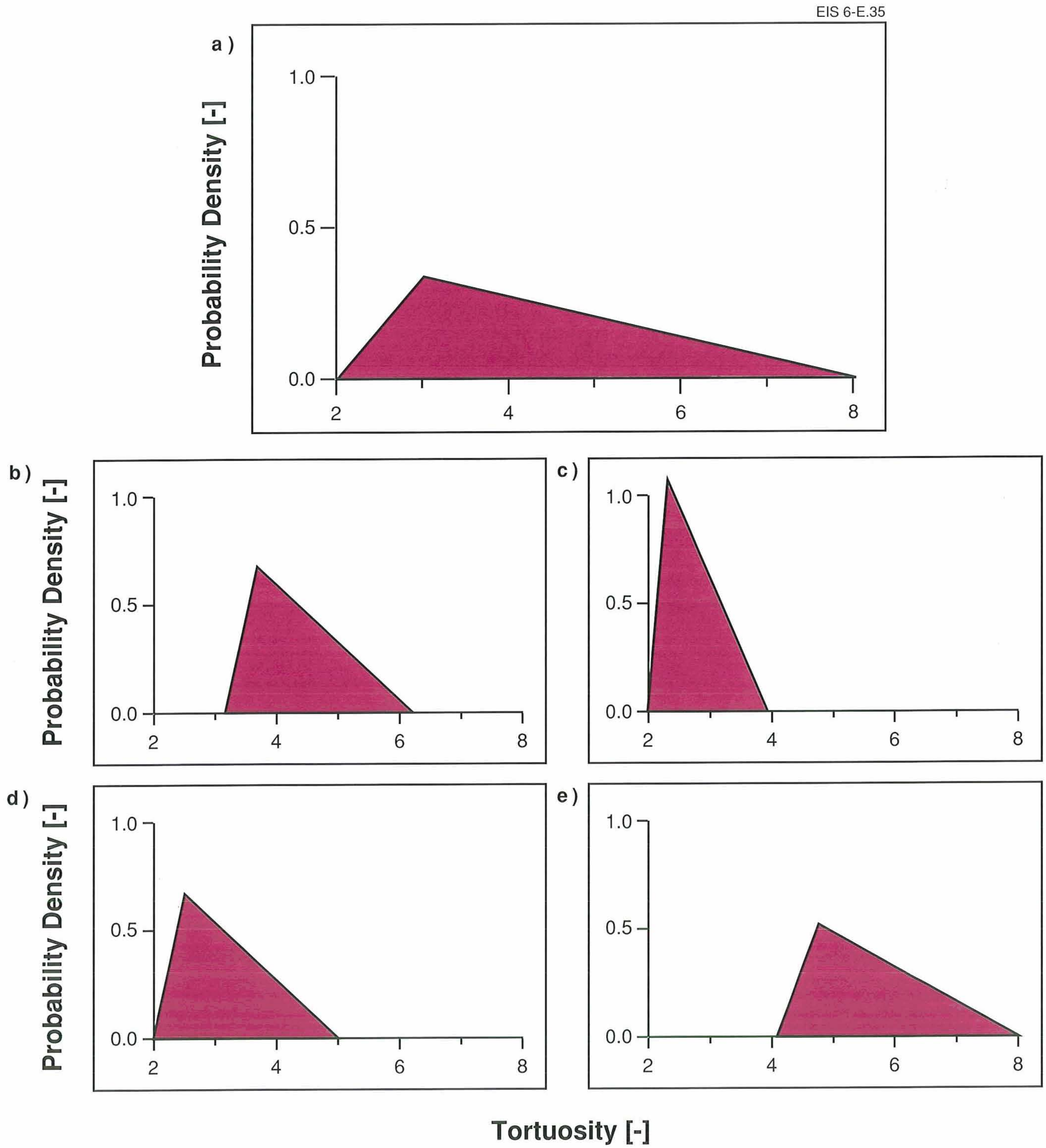


FIGURE E-35: Probability Density Functions for Tortuosity

In the probabilistic analysis of the reference disposal system, the tortuosity of the lower rock zone (a dimensionless parameter) is characterized by a triangular PDF, with values ranging from 2.0 to 8.0. It is shown as PDF A in this figure. PDFs B to E are variants of PDF A that are examined in this section. Table E-6 lists the attributes of these PDFs.

TABLE E-6

ATTRIBUTES OF PDFS FOR TORTUOSITY AND EFFECTS ON THE MEAN OF THE MAXIMUM ANNUAL DOSE ESTIMATES*

PDF	PDF Attributes** Lower Bound	Mode	Upper Bound	Mean	Mean Maximum Annual Dose (Sv/a)	95% Confidence Bounds (Sv/a)
A	2.00	3.00	8.00	4.33	1.2×10^{-6}	$\pm 0.43 \times 10^{-6}$
B	3.17	3.67	6.17	4.33	0.53×10^{-6}	$\pm 0.13 \times 10^{-6}$
C	2.00	2.32	3.89	2.74	4.3×10^{-6}	$\pm 0.87 \times 10^{-6}$
D	2.00	2.50	5.00	3.17	2.8×10^{-6}	$\pm 0.67 \times 10^{-6}$
E	4.11	4.77	8.00	5.63	0.14×10^{-6}	$\pm 0.045 \times 10^{-6}$

* Each of the five different PDFs is used in sets of 500 simulations in which all parameters (except tortuosity) are given the same sequence of 500 randomly sampled values. The tortuosity is sampled from one of the five PDFs in each set of 500 simulations. The results are used to calculate the mean of the maximum ADES from ^{14}C and ^{129}I to 10^5 a. The last column shows the 95% confidence bounds (Section A.3.5 in Appendix A) of the mean of the maximum ADES for each set.

** The tortuosity of the lower rock zone is described using a triangular PDF for the reference disposal system. Each of PDFs A to E is a triangular PDF with the characteristics shown above. The attributes of a triangular PDF, or the parameters used to completely define the distribution, are the lower and upper bounds and the mode (or most probable value). The mean value is calculated from the three PDF attributes. Probability density function A is the PDF of the tortuosity of the lower rock zone used in the analysis of the reference disposal system. PDFs B through E are variants examined in this study. Their attributes are listed in this table, with plots shown in Figure E-35.

Figure E-36 shows a pairwise comparison of each of the 500 simulations corresponding to PDFs B and D. In the scatter plot, the maximum ADEs for PDF B are plotted in the horizontal direction, with each corresponding maximum ADEs for PDF D plotted in the vertical direction. If there were no differences between the two sets of simulations, the points would plot on the diagonal line. This is not the case; the points are asymmetrically positioned with respect to the diagonal such that the maximum ADEs using PDF D are always larger than those using PDF B. This result follows from two considerations:

- The mean value of the tortuosity for PDF B is about 36% larger than that for PDF D; with the sampling scheme used, values of the tortuosity using PDF B are always larger than the values using PDF D.

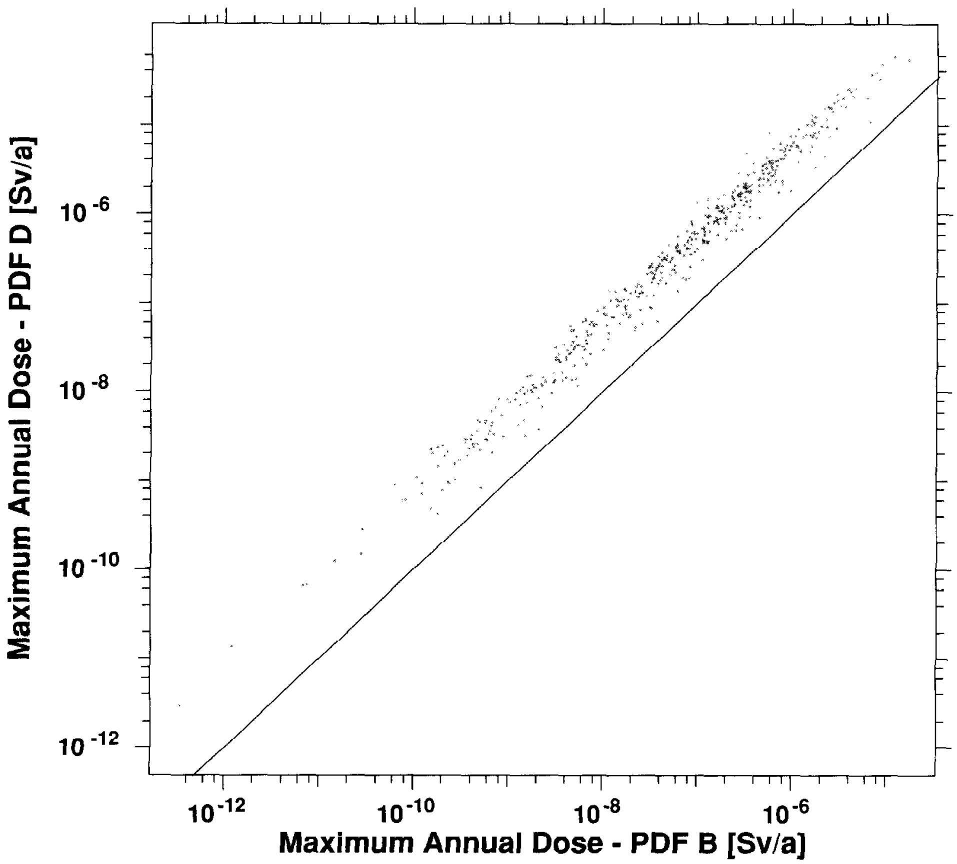


FIGURE E-36: Pairwise Comparisons Involving PDF B and PDF D

This scatter plot compares results from two sets of 500 simulations where the results are the maximum ADEs for times up to 10^5 a. Each symbol represents a pair of simulations in which all parameters have identical values (which are randomly sampled from the PDFs used in the probabilistic analysis), except for the tortuosity of the lower rock zone. The values sampled for tortuosity are also randomly sampled, but use PDFs B or D (Table E-6 and Figure E-35). These two PDFs have identical widths, but PDF B is shifted toward greater values. The sampling scheme is such that the value of the tortuosity of the lower rock zone is greater by 1.17 for every pair of simulations when using PDF B.

The maximum ADEs using PDF B are plotted along the horizontal axis, whereas the corresponding estimates using PDF D are plotted along the vertical axis. If the tortuosity had no effect, the points would plot on the diagonal line. In every simulation, however, the maximum ADE is greater when using PDF D, demonstrating that these estimates are very sensitive to the tortuosity of the lower rock zone.

- Previous sensitivity analysis studies have shown that the maximum ADE is negatively correlated with tortuosity. That is, smaller values of tortuosity lead to greater transport of radionuclides, and thus to greater estimates of annual dose.

Table E-6 shows that the mean of the maximum ADEs is about 5 times greater when using PDF D, compared with PDF B. That is, the maximum ADE is very sensitive to the location of the mode (or mean) of the PDF for the tortuosity of the lower rock zone: a 36% increase in the mean of the tortuosity would decrease the mean of the maximum ADEs by more than 80% at 10^5 a.

E.7.3 EFFECTS OF CHANGING THE WIDTH OF A PDF

We can also quantify the relationship between the uncertainty in the tortuosity and the effects on ADE. We examine here the effects of the width of the PDF for tortuosity of the lower rock zone on the confidence limits on the mean of the maximum ADEs. Figure E-37 shows the relative uncertainty in the mean of the maximum ADEs plotted against the width of the PDF (upper bound minus lower bound). The relative uncertainty is calculated using

$$\frac{\text{upper 95\% confidence bound - lower 95\% confidence bound}}{\text{mean of the maximum ADEs}}$$

with the data in Table E-6.

The points produced by evaluating these ratios for each PDF are well represented by the straight line shown in Figure E-37. It shows that the relative uncertainty in the mean of the maximum ADEs increases in proportion to an increase in the uncertainty of the tortuosity of the lower rock zone.

If we extend the line in Figure E-37 to the zero-width value, the corresponding relative uncertainty left in the mean of the maximum ADEs is about 0.25 (not shown in the figure). That is, if we remove all the uncertainty in the value of the tortuosity of the lower rock zone, we also remove about 75% of the uncertainty in the mean of the maximum ADEs. The remaining 25% of the uncertainty is induced by the range of possible values of the other system parameters. Thus this analysis suggests that substantial reductions in uncertainty would occur with reduced uncertainty in the tortuosity of the lower rock zone.

E.7.4 SUMMARY OF PDF CHANGES

Figure E-38 summarizes the effect on the mean of the maximum ADEs when the PDF is changed. It plots

- the mode, mean and width (upper bound minus lower bound) for each simulation PDF along the horizontal axis, and

- the logarithm of the mean of the maximum ADEs and its 95% confidence bounds along the vertical axis.

It is clear that the mean of the maximum ADEs decreases as the mean and mode of the PDF increase.

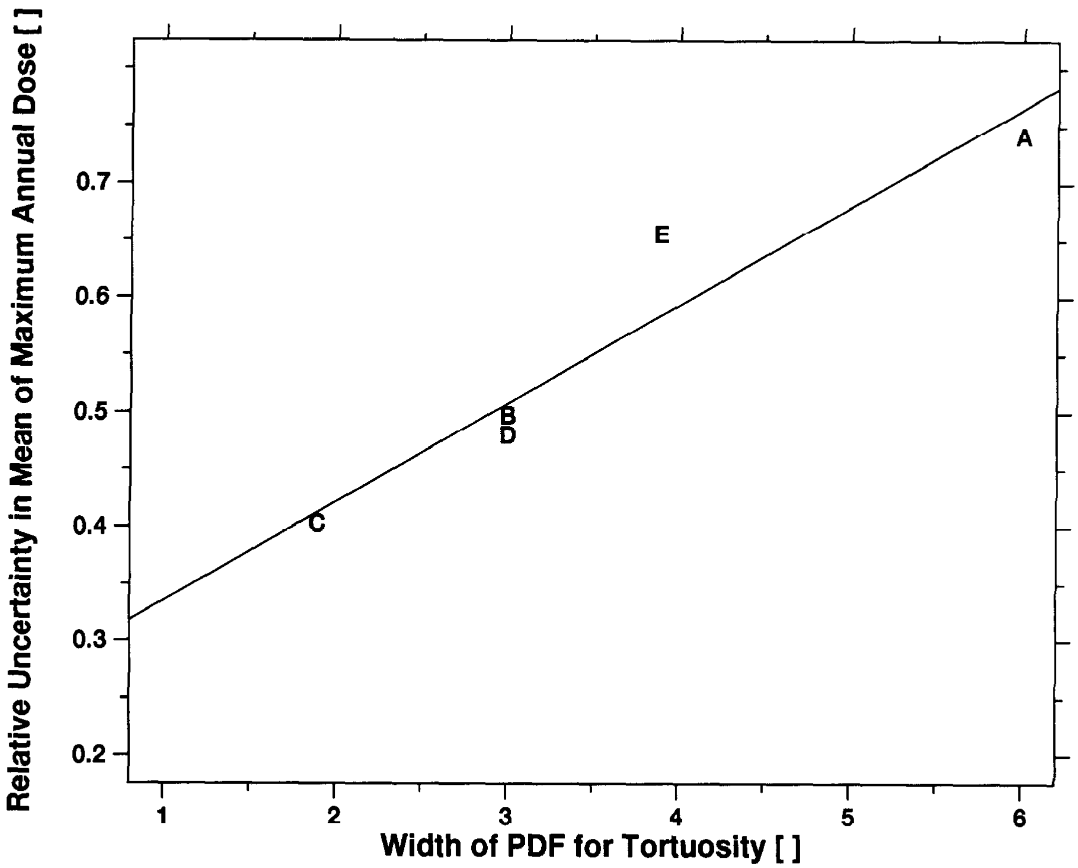


FIGURE E-37: Relative Uncertainty in the Mean of the Maximum Annual Dose Versus Width of the PDF

The vertical axis in this plot is the relative uncertainty in maximum ADE, defined by the expression:

$$\frac{\text{upper 95\% confidence bound} - \text{lower 95\% confidence bound}}{\text{mean of the maximum annual dose estimate}}$$

and uses data from Table E-6. The horizontal axis is the width of the PDFs used in this study for the tortuosity of the lower rock zone. The width of a triangular PDF is equal to the difference between its upper and lower bounds. The results demonstrate that the uncertainty in the maximum annual dose increases as the uncertainty in the PDF for tortuosity increases.

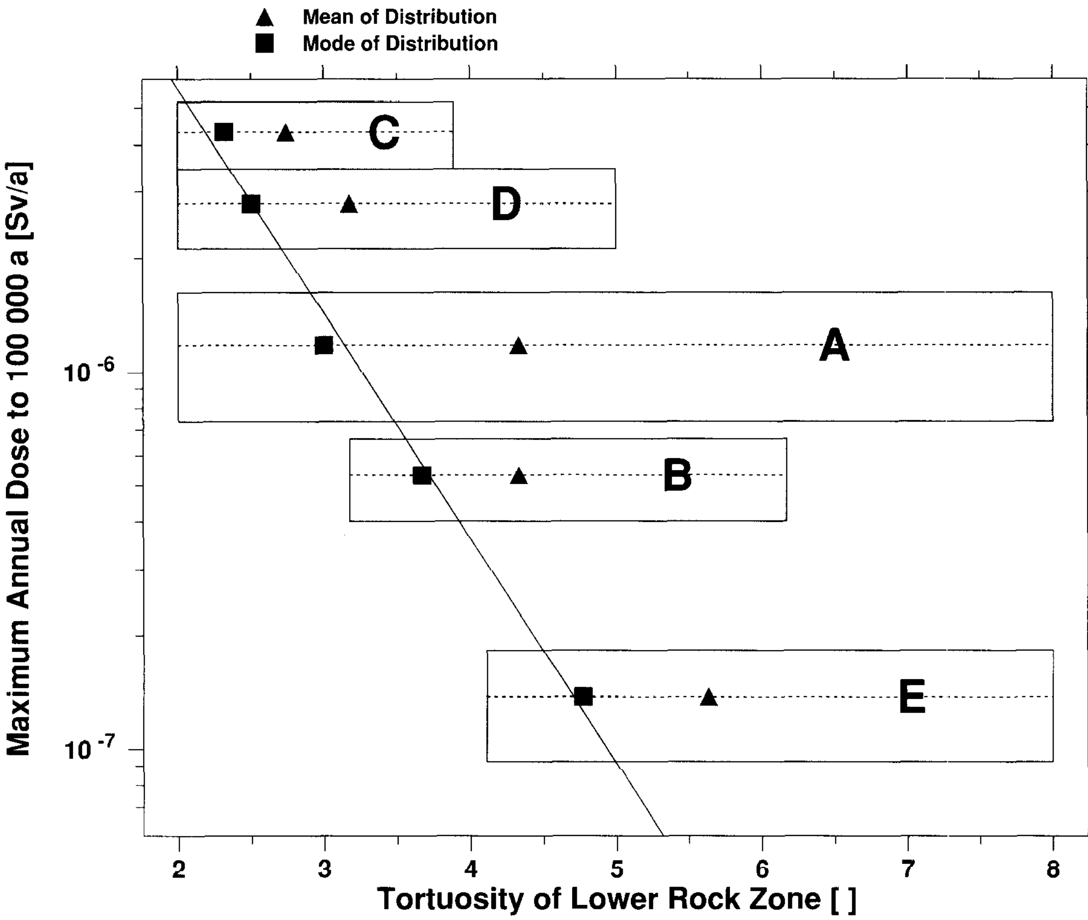


FIGURE E-38: Mean of the Maximum Annual Dose Estimates Versus Tortuosity of the Lower Rock Zone

The vertical axis uses a logarithmic scale and plots the arithmetic average from 500 simulations of the maximum ADEs to 10^5 a. The horizontal axis shows values of the tortuosity of the lower rock zone (a dimensionless parameter). The data are for the five PDFs in Table E-6. For each PDF

- the dashed horizontal line shows the mean value of the maximum ADEs,
- the solid lines above and below the mean value show the corresponding 95% confidence bounds,
- the symbols on the dashed horizontal line locate the mode and mean value of the tortuosity of the lower rock zone, and
- the solid vertical lines delineate the PDF width.

The diagonal line is a regression line, which suggests that a linear relationship exists between the mode of the tortuosity and the logarithm of the mean of the maximum ADEs.

We can quantify a relationship for the data in this figure between the mean of the maximum ADEs and the mode of the tortuosity of the lower rock zone. The diagonal regression line in Figure E-38 suggests that the logarithm of the mean of the maximum ADEs is approximately proportional to the value of the mode of the test PDFs.

This linear relationship has further implications regarding the overall safety of the reference disposal system. The largest value in the mean of the maximum ADEs would be obtained when the tortuosity takes on small values. Tortuosity is a measure of the increase in diffusive transport pathway caused by the tortuous nature of the water-filled spaces that contaminants follow during their movement. Its physical lower bound is unity, corresponding to diffusive transport in free water. For any geological medium, this lower bound must be greater; for example, a value of 1.4 would be typical for loose sand.

The minimum possible value for the tortuosity of the lower rock zone is 2.0, corresponding to the shortest possible diffusive path (and shortest travel time) for contaminants exiting the vault. Using this value, Figure E-38 shows the corresponding maximum annual dose up to 10^5 a is about 6×10^{-6} Sv/a, smaller than the annual dose limit associated with the AECB risk criterion. In other words, this analysis implies that even the use of the most unfavourable value of the tortuosity of the lower rock zone would result in a mean of the maximum ADEs that would still be below a dose limit of 5×10^{-5} Sv/a. This implication must be used with caution because it is based on an extrapolation of results to a value of tortuosity that is beyond its specified range and because it assumes that this value of the tortuosity would remain consistent with other parameters describing the characteristics of the lower rock zone.

The analysis described above leads to a specific conclusion:

- it would be worthwhile to conduct further research studies aimed at quantification of the tortuosity of the lower rock zone. Changes to the width and mode of its triangular PDF would have significant effects on both the magnitude and relative uncertainty in the mean of the maximum ADEs. (By implication, the use of different types of PDFs and different ranges of permitted values are also expected to have significant effects.)

We can generalize this conclusion somewhat. As noted earlier, the tortuosity of the lower rock zone is one of several interrelated parameters used to describe contaminant transport in the rock surrounding the vault; other parameters include permeability, porosity, the types and amounts of minerals present, and the length of the waste exclusion distance. Our analysis, therefore, supports the more general conclusion:

- it would be worthwhile to continue research studies aimed at better quantification of contaminant transport in the sparsely fractured low-permeability rock of the lower rock zone.

E.8 DETAILED ANALYSIS OF THE EFFECTS OF SELECTED SITE AND DESIGN FEATURES

E.8.1 INTRODUCTION

Section 6.6 in the main text summarizes the results of special sensitivity analyses focussed on

- the effects of potential design constraints that could improve the estimated performance of the reference disposal system; and

- the influence of different assumed values for selected site features.

The analyses use similar sets of 500 simulations. The reference set corresponds to the first 500 randomly sampled simulations in the analysis of the reference disposal system. For each other set, most parameters take on the identical sequence of 500 randomly sampled values, and one parameter (or possibly several related parameters) uses a value chosen to display the effects of an assumed site or design feature.

The calculated variables compared are arithmetic means of maximum ADEs:

- Table 6-16 and Figures 6-24 and 6-25 in the main text show the results for the total ADEs resulting from seven radionuclides (^{14}C, ^{135}Cs, ^{129}I, ^{59}Ni, ^{107}Pd, ^{79}Se and ^{99}Tc from used fuel). Of these, only ^{14}C and ^{129}I are major contributors to dose in the analysis described in Sections 6.2 to 6.5 in the main text. In the following results, ^{99}Tc makes a small contribution in some simulations.

- Table 6-17 in the main text and Figures E-39 to E-41 show the results for the ADEs resulting from ^{14}C, ^{129}I and ^{99}Tc. A comparison of these results shows that some assumed site and design features are more influential for different radionuclides.

The remainder of this section provides a detailed discussion of the results of the analysis, including examination of the reasons for the different effects. The cases studied are the 13 listed in Table 6-15 in the main text. Section 6.6.3 in the main text summarizes the results.

E.8.2 CASE 1 - INCREASED CONTAINER WALL THICKNESS

The effective thickness (or corrosion allowance) of the wall of the titanium containers in the reference disposal system is 4.2 mm (Johnson et al. 1994). In Case 1, we assume an effective thickness of 8.4 mm, a potential design constraint that might be achieved by re-designing the container with corresponding allowances in the boreholes in the vault.

The extra thickness increases the time required for corrosion processes to breach the container, and thus delays the release of contaminants. For most simulations, breakthrough of ^{129}I to the biosphere is just beginning near 10^4 a for many simulations, and the additional delay reduces estimated

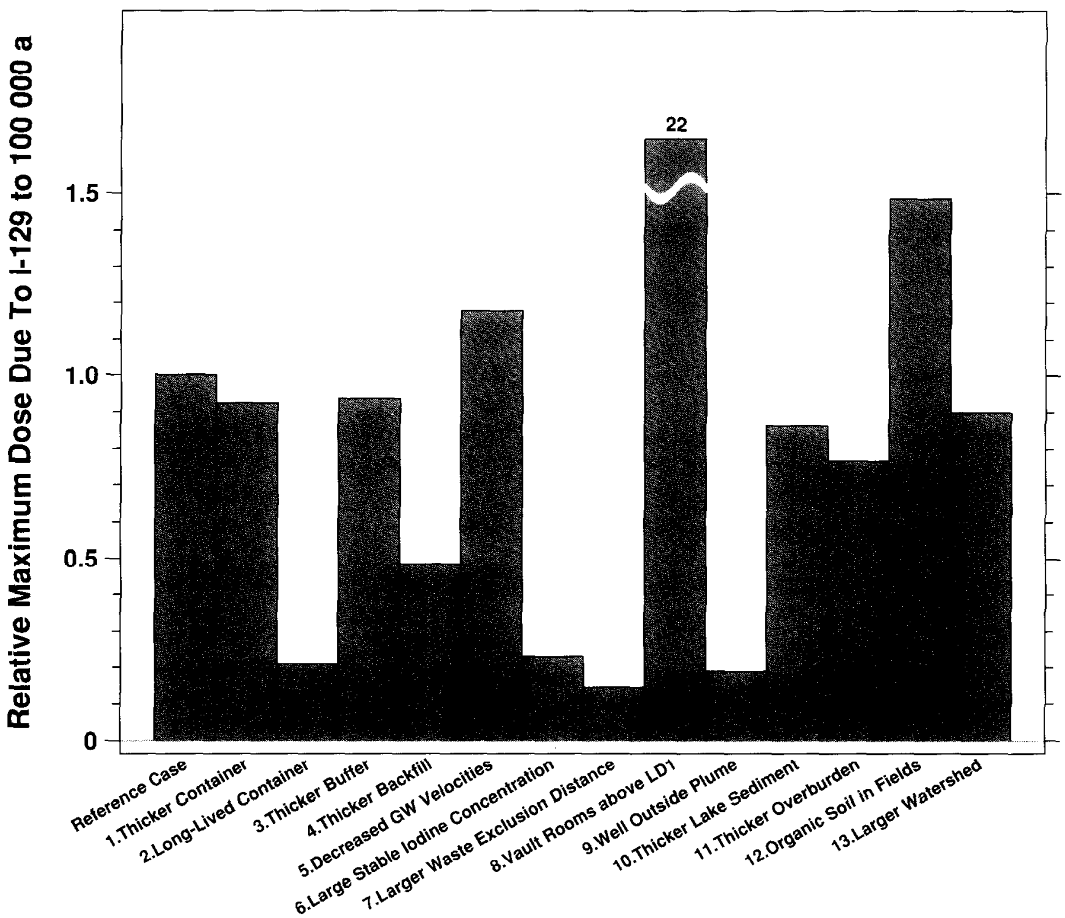


FIGURE E-39: Effects of Assumed Site or Design Features on the Mean of the Maximum Annual Dose Estimates from ^{129}I

These results are computed from estimates of annual dose from ^{129}I from similar sets of 500 randomly selected simulations. The plots are shown relative to a reference case, shown as the first bar on the left-hand side. The reference case corresponds to the mean of the maximum (up to 10^5 a) ADES resulting from ^{129}I from the first 500 random simulations of the reference disposal system. Each other bar shows the effects of an assumed site or design feature.
Cases 7 and 9 show the greatest decrease in the mean of the maximum ADEs; Case 8 shows the greatest increase (note that the top of the bar for Case 8 extends to 22, beyond the scale of the vertical axis). Data for this figure are taken from Table 6-17 in the main text.

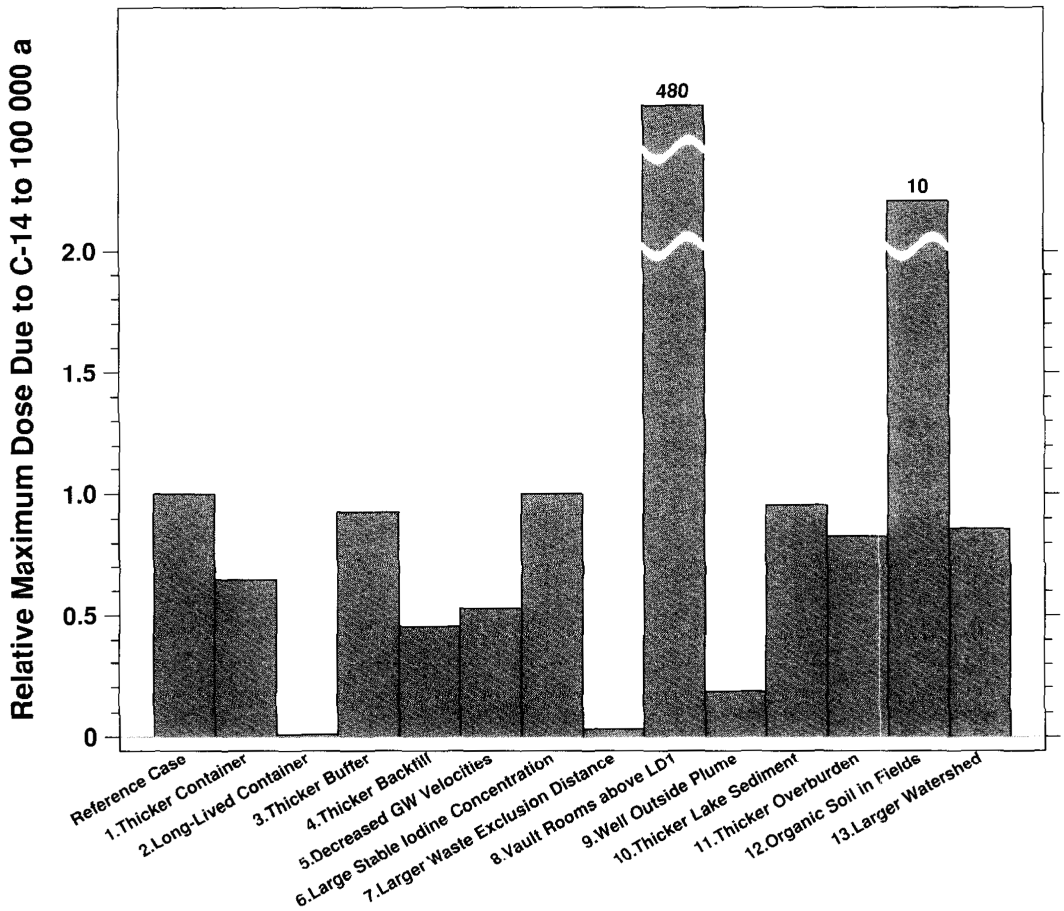


FIGURE E-40: Effects of Assumed Site or Design Features on the Mean of the Maximum Annual Dose Estimates from ^{14}C

These results are computed from estimates of annual dose from ^{14}C from similar sets of 500 randomly selected simulations. The plots are shown relative to a reference case, shown as the first bar on the left-hand side. The reference case corresponds to the mean of the maximum (up to 10^5 a) ADEs resulting from ^{14}C from the first 500 random simulations of the reference disposal system. Each other bar shows the effects of an assumed site or design feature.
Cases 2 and 7 show the greatest decrease in the mean of the maximum ADEs; Case 8 shows the greatest increase (note that the top of the bar for Case 8 extends to 480, far beyond the scale of the vertical axis). Data for this figure are taken from Table 6-17 in the main text.

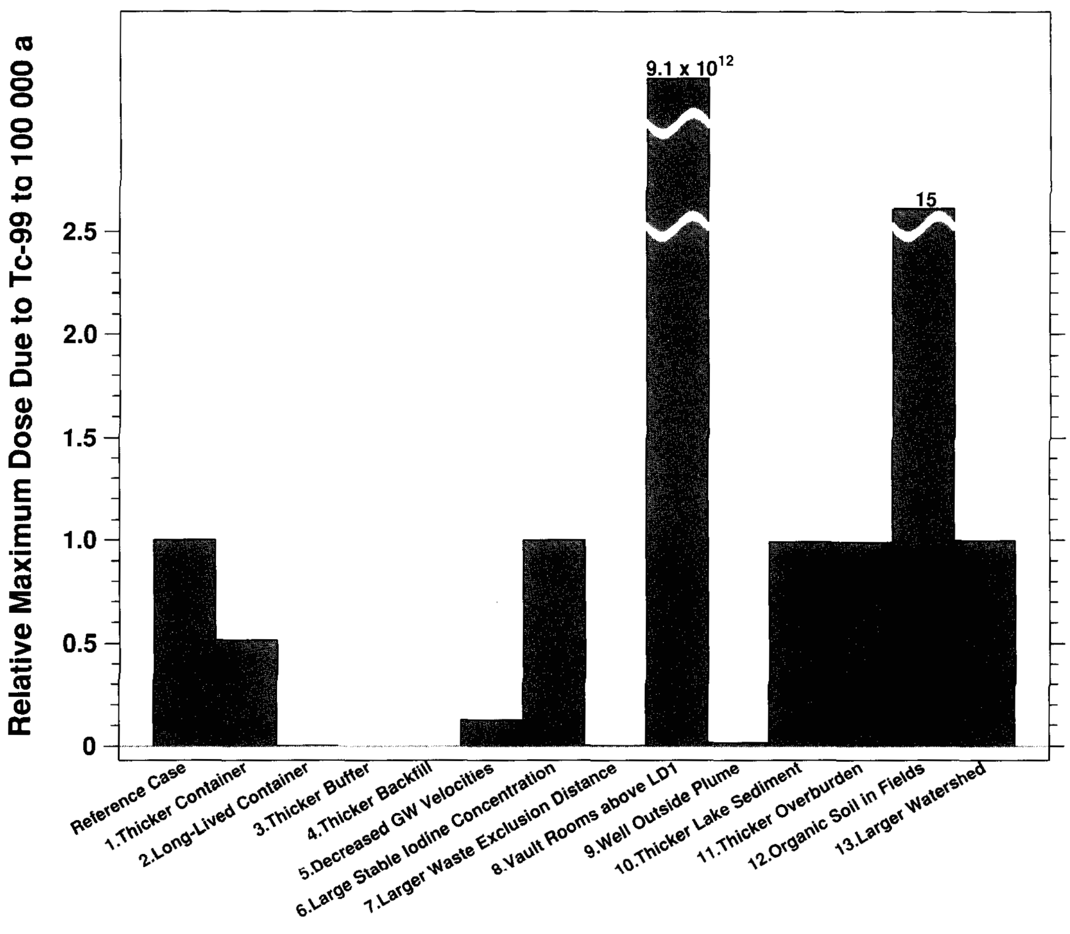


FIGURE E-41: Effects of Assumed Site or Design Features on the Mean of the Maximum Annual Dose Estimates from ^{99}Tc

These results are computed from estimates of annual dose from ^{99}Tc from similar sets of 500 randomly selected simulations. The plots are shown relative to a reference case, shown as the first bar on the left-hand side. The reference case corresponds to the mean of the maximum (up to 10^5 a) ADEs resulting from ^{99}Tc from the first 500 random simulations of the reference disposal system. Each other bar shows the effects of an assumed site or design feature.
Cases 2, 3, 4, 7 and 9 show large decreases in the mean of the maximum ADEs; Case 8 shows an extremely large increase (note that the top of the bar for Case 8 extends to 9.2×10^{12}, many orders of magnitude beyond the scale of the vertical axis). Data for this figure are taken from Table 6-17 in the main text.

releases and the mean ADEs (which is dominated by ^{129}I) by a factor of about 4 (Table 6-16 in the main text). By 10^5 a, ^{129}I releases are not changing as rapidly as a function of time between most simulations, thus there is little effect of changes in delay time on the mean ADE or the maximum ADEs resulting from ^{129}I. Consequences resulting from ^{14}C are more affected than ^{129}I (Table 6-17 in the main text and Figures E-39 and E-40) at 10^5 a because the extra delay time allows radioactive decay to attenuate the peak. Consequences resulting from ^{99}Tc are also more affected than ^{129}I (Table 6-17 in the main text and Figures E-39 and E-41) because ^{99}Tc is just starting its breakthrough to the biosphere at 10^5 a.

Figure E-42 shows a pairwise comparison of each of the 500 simulations from Case 1 with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At 10^4 a, only some of the simulations are affected by this parameter change; at 10^5 a there is little or no effect on any of the simulations.

E.8.3 CASE 2 - MORE DURABLE CONTAINER

In the reference disposal system, some containers fail within 50 a, and the median lifetime is about 4000 a (Johnson et al. 1994). In Case 2, we assume that the containers are more durable. Container corrosion parameters have been adjusted so that no containers fail before 10^4 a, and the median container lifetime is about 10^5 a. The thick copper containers described in the Swedish concept (SKBF 1983) are even more durable than those in this case.

The ADE is zero at 10^4 a (Table 6-16 in the main text) because no containers fail before this time. The differential effects on ^{129}I compared with ^{14}C and ^{99}Tc (Table 6-16 in the main text and Figures E-39 to E-41) can be attributed to the extra delay afforded by the durable containers, similar to the effects described in Case 1. The effects are greater than in Case 1 because the delay is longer.

Figure E-43 shows a pairwise comparison of each of the 500 simulations from this case with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At 10^4 a every simulation involving the more durable container has a value of zero for the ADE; at 10^5 a every simulation has substantially reduced ADEs.

E.8.4 CASE 3 - THICKER BUFFER

The buffer thickness in the reference disposal system is 0.25 m (Johnson et al. 1994); in this study it is assumed to be 1.0 m. This design constraint might be achieved by redesigning the boreholes in the vault, or by changing the design to an "in room" emplacement concept (such as that assessed by Wuschke et al. (1981, 1985)).

The extra thickness of the buffer increases the time required for the transport of contaminants from the container to the surrounding media. It is particularly effective for contaminants such as ^{99}Tc (Table 6-17 in the main text and Figure E-41) that are sorbed onto the buffer material. It is much less effective for contaminants that do not sorb onto buffer, such as ^{14}C and ^{129}I.

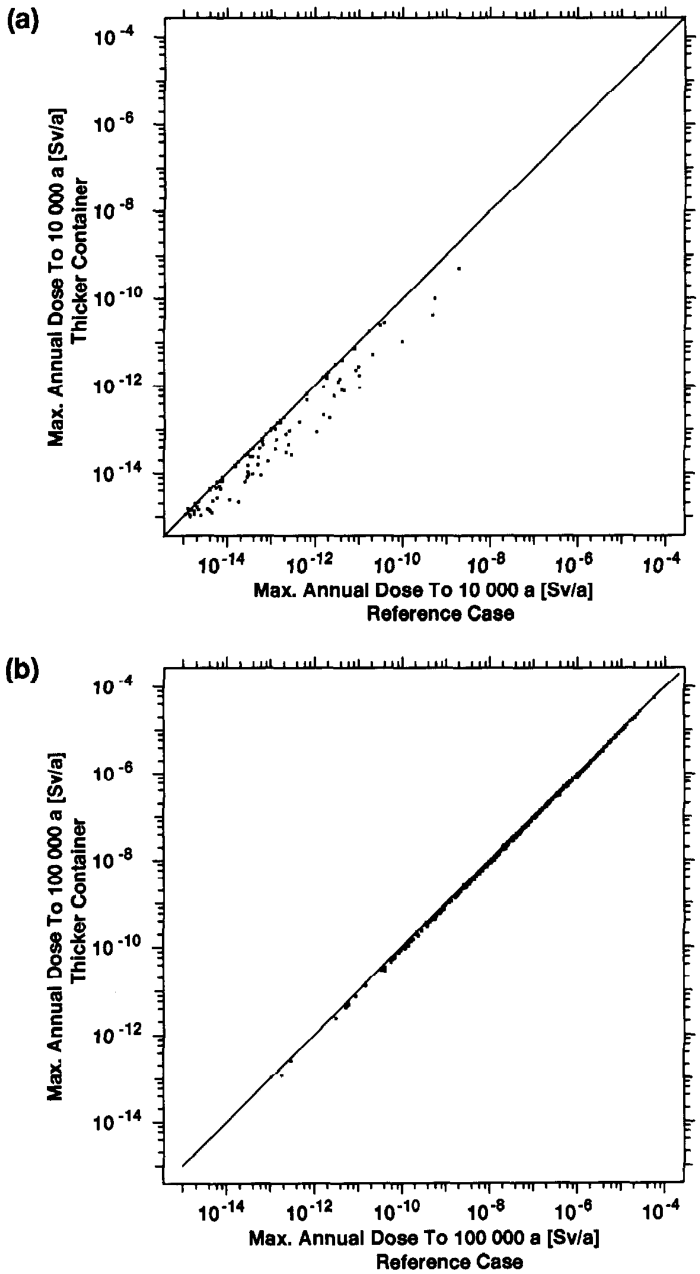


FIGURE E-42: Effect of Increased Container Wall Thickness

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical except for the thickness of the container. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations with an assumed increase in container thickness. Points falling on the diagonal line indicate pairs of simulations with identical results.

The increased container thickness leads to smaller maximum ADEs in every simulation, although the differences are small at 10^5 a.

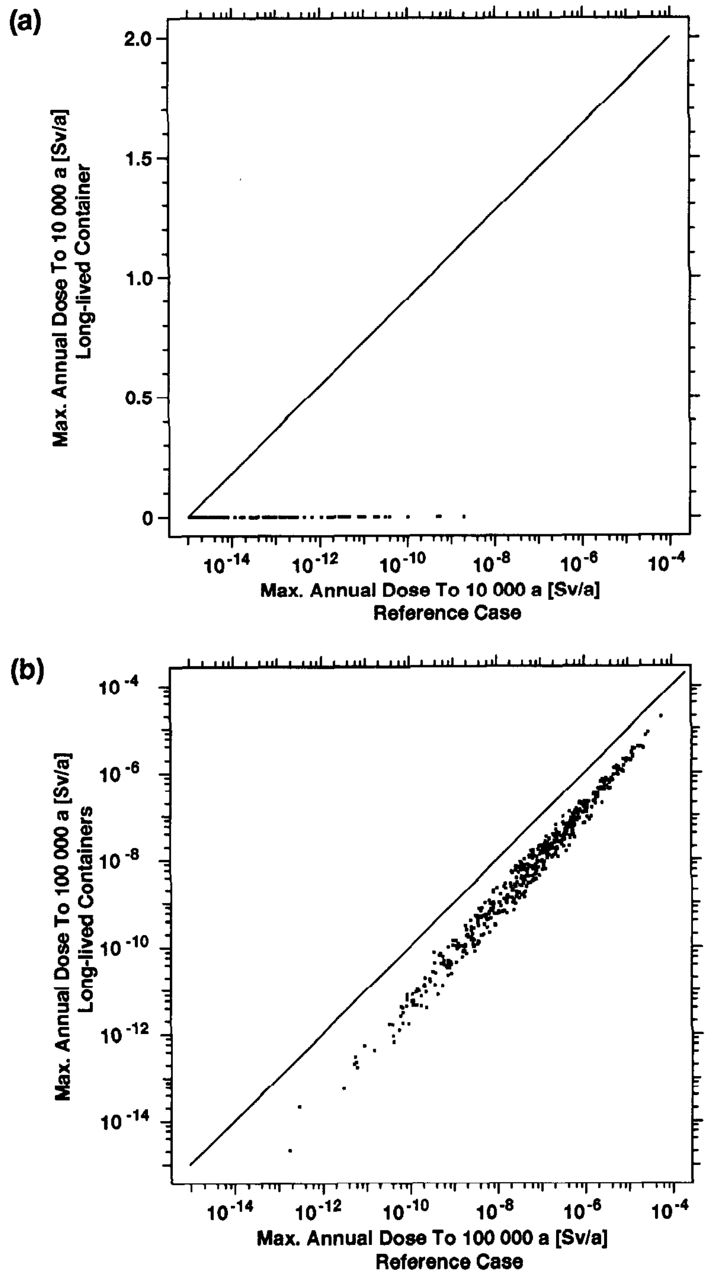


FIGURE E-43: Effect of More Durable Containers

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical except for the durability of the containers. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations that assume no containers fail before 10^4 a. Points falling on the diagonal line indicate pairs of simulations with identical results. Part (a) uses a linear vertical scale to confirm ADEs are zero before 10^4.
The more durable containers essentially eliminate radiation doses at 10^4 a and are still effective at 10^5 a.

Figure E-44 shows a pairwise comparison of each of the 500 simulations from this case with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At both 10^4 a and 10^5 a, most of the simulations are unaffected by this parameter variation, but a few have reduced ADEs. The simulations with largest ADEs are unaffected, and thus the mean ADEs are not much affected.

E.8.5 CASE 4 - THICKER BACKFILL

The effective thickness of the backfill in the reference disposal system is 1.4 m (Johnson et al. 1994); in this study it is assumed to be 2.8 m. This design constraint might be achieved by re-designing the vault to provide more room for backfill material.

The extra thickness of the backfill increases the time required for the transport of contaminants to the rock surrounding the vault. It is particularly effective for contaminants such as ^{99}Tc that are sorbed on the backfill material (Table 6-17 in the main text and Figure E-41). It is also more effective than the buffer for nonsorbing contaminants because the larger porosity of the backfill gives it a greater capacity for holding contaminants.

Figure E-45 shows a pairwise comparison of each of the 500 simulations from this case with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At both 10^4 a and 10^5 a, the thicker backfill reduces the ADE in every simulation by about the same amount.

We also examined a variant of this case, in which we assume there is no backfill in the contaminant pathway. We observe that, if no backfill is present, the mean ADE increases by about 1 order of magnitude at 10^5 a; thus the backfill is an effective barrier for the reference disposal system. Note that this variant cannot be considered as a viable design option because the excavation openings will be filled and because detailed modelling has shown the contaminant plume will penetrate the backfill (Garisto and LeNeveu 1991).

E.8.6 CASE 5 - DECREASED GROUNDWATER VELOCITIES

To study the effect of groundwater velocity in the rock, the PDF for the groundwater velocity scaling factor was assumed to be smaller, so that velocities in all geosphere segments in all simulations were decreased by a factor of 2 compared with the reference disposal system simulations. For example, the groundwater velocity in fracture zone LD1 has a median value of about 0.5 m/a in Case 5, compared with a median value of about 1.0 m/a in the reference disposal system (Davison et al. 1994). This change is not consistent with current information on the WRA and, therefore, cannot be used to improve the performance of the reference disposal system.

The results from this case show mixed effects; for example, the mean ADE is smaller at 10^4 a but larger at 10^5 a (Table 6-16 in the main text). This pattern can be explained with reference to the network of segments in the geosphere, including those leading to the well:

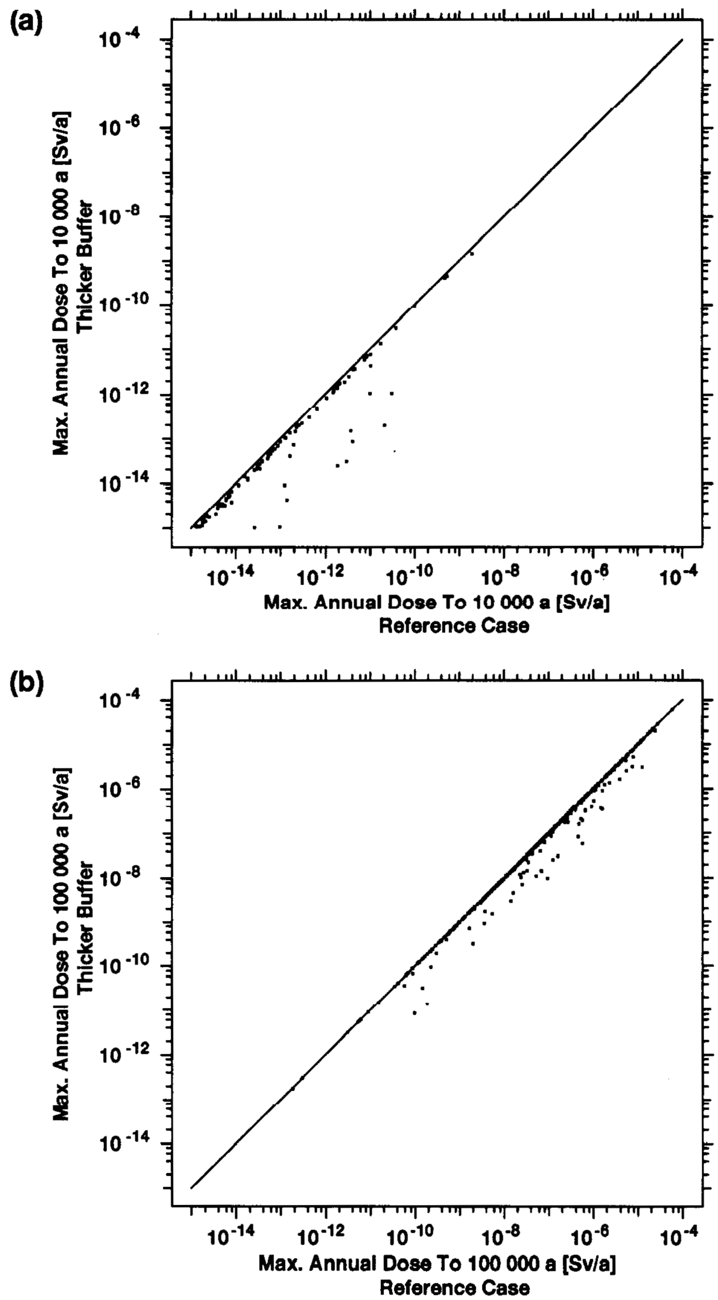


FIGURE E-44: Effect of Increased Buffer Thickness

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical, except for the thickness of the buffer. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations with an assumed increase in buffer thickness. Points falling on the diagonal line indicate pairs of simulations with identical results.

The thicker buffer leads to smaller maximum ADEs for some simulations and is most effective at 10^4 a.

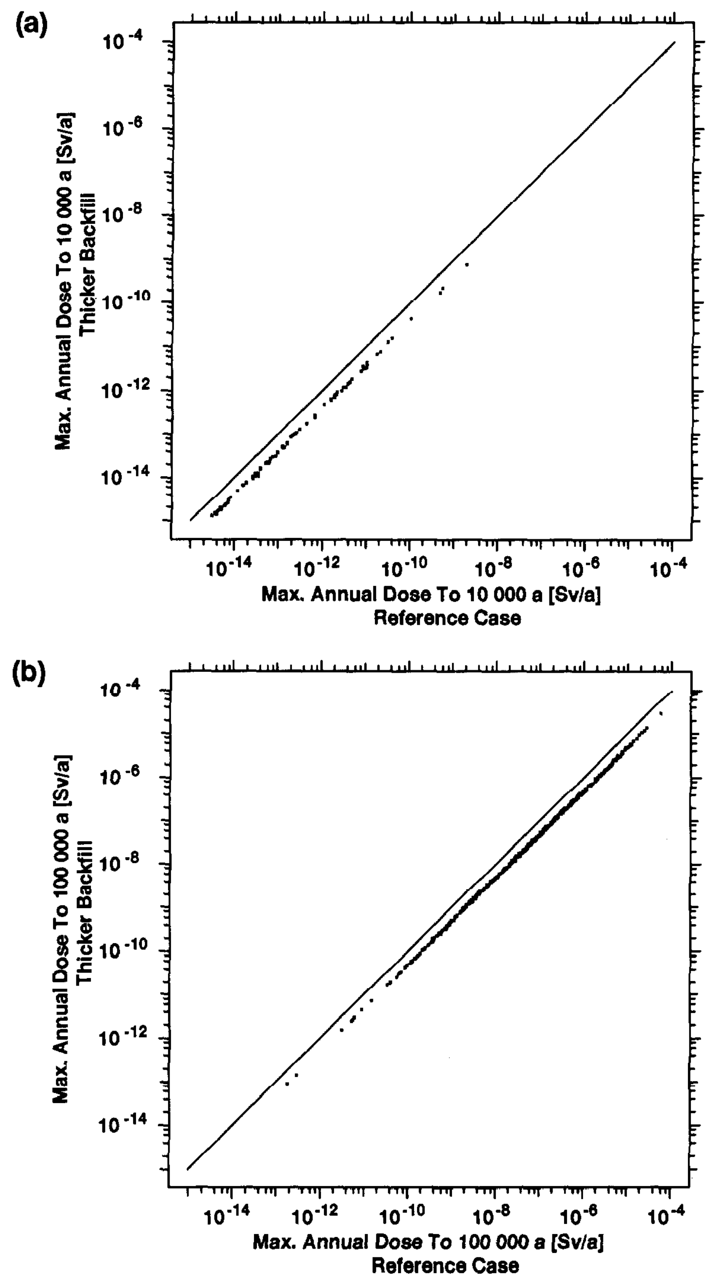


FIGURE E-45: Effect of Increased Backfill Thickness

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical except for the thickness of the backfill. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations with an assumed increase in backfill thickness. Points falling on the diagonal line indicate pairs of simulations with identical results.

For all simulations, the thicker backfill leads to about the same decrease in maximum ADEs at 10^4 and 10^5 a.

- The mean ADE is smaller at 10^4 a in Case 5 because the lower groundwater velocity has reduced the transport of contaminants along all geosphere segments. Breakthrough to the biosphere is just beginning for ^{129}I and ^{14}C near 10^4 a. With lower groundwater velocities, the slower transport results in lower contaminant releases to the biosphere, and thus smaller ADEs, resulting from delay of the breakthrough front.

- The mean ADE is larger at 10^5 a because of the effects of the well (see Section D.7 in Appendix D). The well demands are identical in the reference disposal system and in Case 5. However, the well in Case 5 must collect water from a larger area to meet this demand because groundwater velocities are lower. Thus, a larger portion of the plume of contaminants is captured. Another way to consider this situation is that, with lower groundwater velocities, there is less dilution and, therefore, contaminant concentrations in groundwater and well water are higher. The net result is that ADEs from long-lived nuclides, such as ^{129}I, are larger (Table 6-17 in the main text and Figures E-39 and E-40). The ADEs from nuclides with relatively short half-lives, such as ^{14}C, are smaller because the extra transport time allows for more decay.

Figure E-46 shows a pairwise comparison of each of the 500 simulations from this case with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At 10^4 a, the simulations with the largest ADEs are slightly affected, although most other simulations show a significantly reduced ADE. A few simulations show an increased ADE. At 10^5 a, the individual simulations show both increases and decreases in the ADEs.

In general, higher groundwater velocities result in lower contaminant concentrations that arrive earlier, whereas lower velocities result in greater concentrations that arrive later (unless half-lives are of the same order or smaller than the travel time). Nevertheless, Figure E-46 shows that the trend in ADEs can be reversed in individual simulations because of the complex interactions between parameters such as well demand, well capacity and plume capture fractions (see Section D.7 in Appendix D).

E.8.7 CASE 6 - INCREASED CONCENTRATIONS OF NATURALLY OCCURRING IODINE

In Section 5.6 in the main text, we note that estimated annual doses from ^{129}I are affected by mixing with stable iodine. Within the food-chain and dose model, our calculations include the effects of stable iodine in groundwaters discharging from the geosphere and entering the drinking water of the critical group.

The concentration of stable iodine is described by a PDF with an average value of 12.5 $\mu g/L$ (Gascoyne and Kamineni 1992, Davis et al. 1993). In Case 6, we adjust the PDF so that the average concentration is increased to 125 $\mu g/L$. This change is not consistent with current information at the site of the hypothetical vault in the Whiteshell Research Area (WRA). (However, concentrations of iodine up to 100 $\mu g/L$ have been found in overburden waters in other parts of the WRA and even larger concentrations

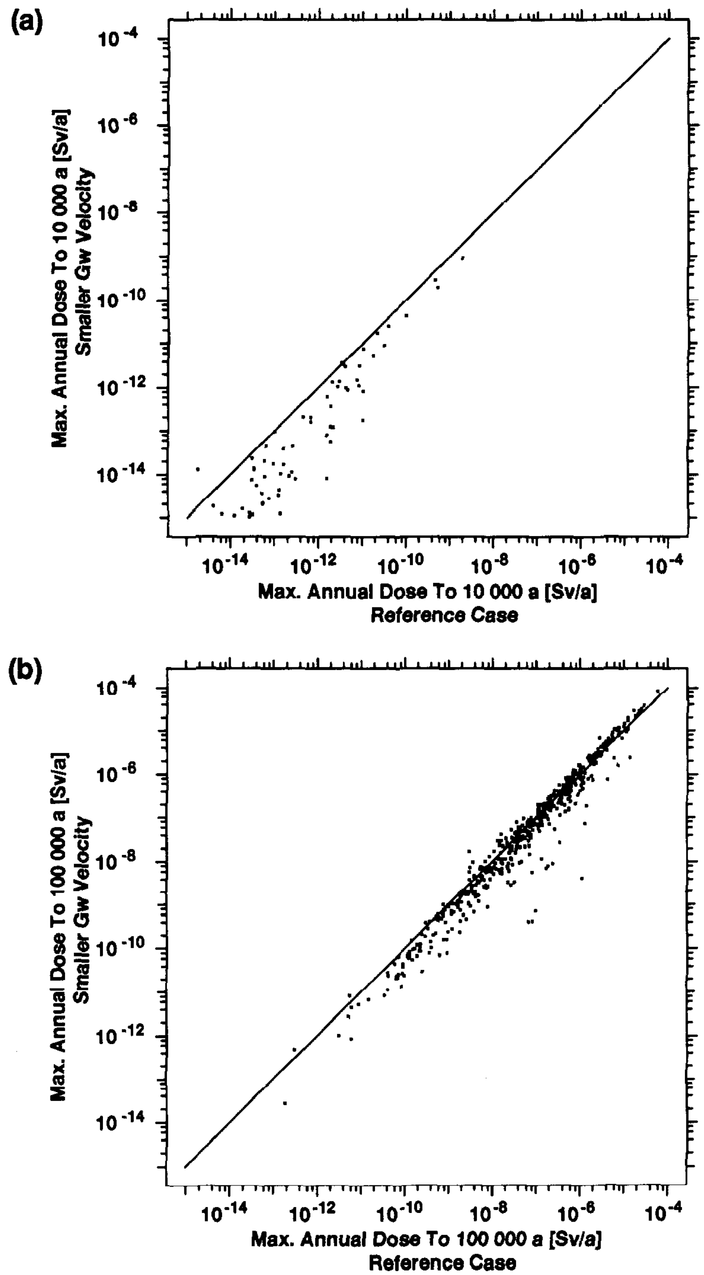


FIGURE E-46: Effect of Reduced Groundwater Velocities

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical except for the assumed groundwater velocities in the geosphere. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations with an assumed smaller groundwater velocity scaling factor (and, therefore, lower groundwater velocities in the geosphere). Points falling on the diagonal line indicate pairs of simulations with identical results.

At 10^4 a, a lower groundwater velocity yields smaller maximum ADEs for almost all simulations because slower transport results in smaller contaminant releases to the biosphere. At 10^5 a, this pattern is reversed for many simulations because of the complex interactions between well demand and fraction of the contaminant plume captured by the well (see text).

of iodine have been observed in other areas of the Canadian Shield (Gascoyne and Kamineni 1992, Frape and Fritz 1987).)

As expected, increasing the concentration of naturally occurring iodine decreases the mean ADE at 10^4 and 10^5 a (Table 6-16 in the main text and Figure E-39) because it reduces ADEs from ^{129}I by isotopic dilution (ADEs from ^{14}C and ^{99}Tc are not affected). The assumed tenfold increase in concentrations of naturally occurring iodine results in a mean ADE reduction of a factor of only 4 to 5 (Table 6-16 in the main text and Figure E-39) because isotopic dilution does not occur in all simulations.

Figure E-47 shows a pairwise comparison of each of the 500 simulations from this case with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At both 10^4 a and 10^5 a, many of the simulations are unaffected by increased concentrations of naturally occurring iodine, whereas others show the effects of up to a tenfold decrease in the ADE. As expected, the simulations with the largest ADEs are more likely to be affected because they also have largest estimated concentrations of ^{129}I.

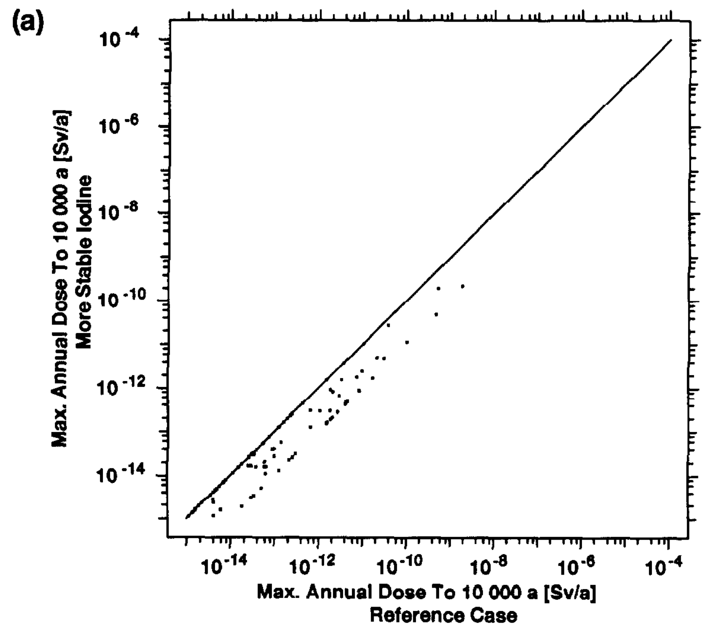
E.8.8 CASE 7 - INCREASED WASTE EXCLUSION DISTANCE

The waste exclusion distance is the layer of rock isolating the waste emplacement part of any vault room from fracture zone LD1 (Section 5.2 in the main text). For the reference disposal system, about 50 m of sparsely fractured rock is between the nearest container and LD1. In Case 7, we examine an increased distance of about 70 m, which increases the lengths of the segments in the geosphere that connect the vault to fracture zone LD1.

This case describes a potential design constraint because it would be achieved by adjusting the vault layout relative to fracture zone LD1. In a more general sense, it might be classified as a site feature related to the number and types of fractures in the host rock surrounding a disposal vault.

The major effect of changes to the waste exclusion distance is on the time required for transport of contaminants from the vault to LD1. The effect on the ADE is more important at early times because only a few radionuclides in a few simulations have broken through to the biosphere. The results in Table 6-16 in the main text show that, at 10^4 a, the ADEs are about 5 orders of magnitude smaller for the 70-m waste exclusion distance. The effects of delay are less significant at 10^5 a because the major contributor to the ADE, ^{129}I, has smaller differences in discharge rates for most simulations. Table 6-17 in the main text and Figures E-39 to E-41 show that the ADEs are more decreased at 10^5 a for ^{14}C and ^{99}Tc than for ^{129}I. This occurs because of the greater extent of radioactive decay of ^{14}C before the peak is released and because of the additional delay of the leading edge of the breakthrough of ^{99}Tc, resulting from the sorption of ^{99}Tc on the additional rock between the vault and LD1.

Figure E-48 shows a pairwise comparison of each of the 500 simulations from this case with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At both 10^4 a and 10^5 a, all the simulations are affected by the increase in waste exclusion distance and show significantly reduced ADEs.



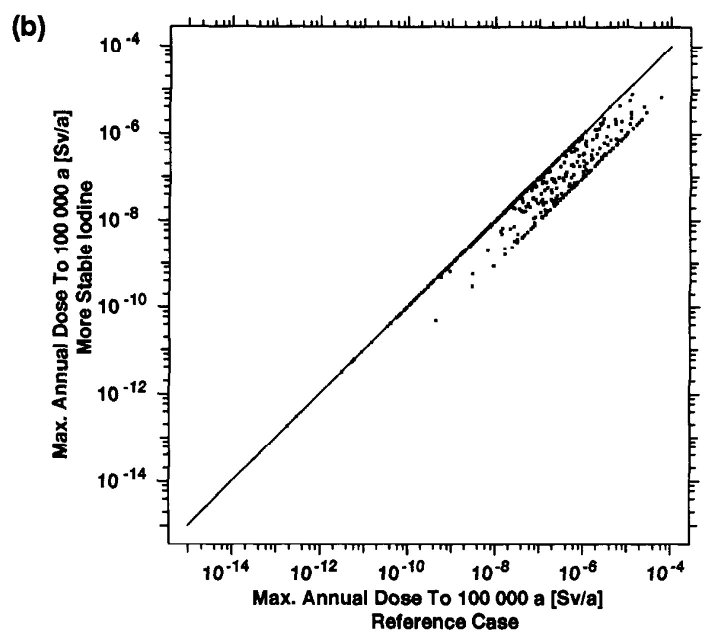


FIGURE E-47: Effect of Increased Concentrations of Naturally Occurring Iodine

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical except for the concentrations of naturally occurring iodine in groundwater. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations with larger assumed concentrations of naturally occurring iodine. Points falling on the diagonal line indicate pairs of simulations with identical results.
Larger assumed concentrations of naturally occurring iodine lead to smaller maximum ADEs, with a maximum reduction of about 10.

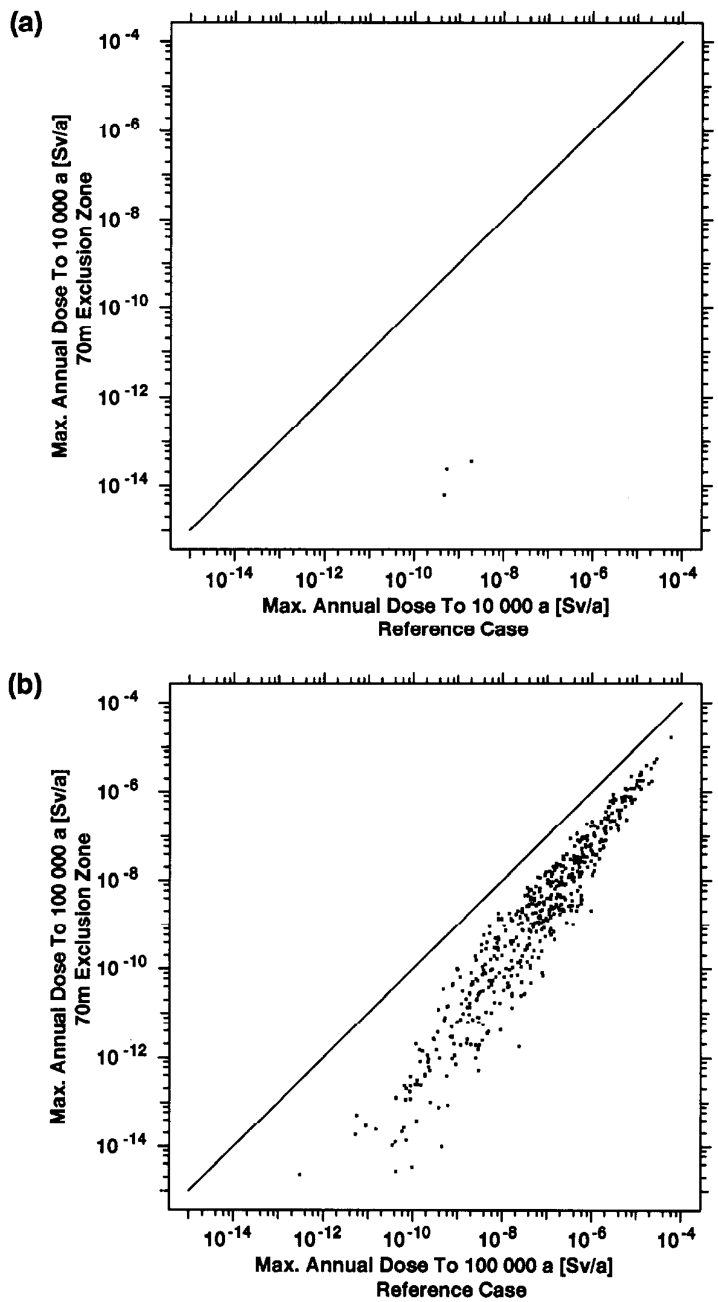


FIGURE E-48: Effect of a Larger Waste Exclusion Distance

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical except for the size of the waste exclusion distance. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system with a 50-metre waste exclusion distance. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations with an assumed waste exclusion distance of 70 m. Points falling on the diagonal line indicate pairs of simulations with identical results.
The larger waste exclusion distance shows large reductions in the maximum ADEs, especially at 10^4 a.

Auxiliary studies have confirmed the importance of the waste exclusion distance:

- For an assumed waste exclusion distance of about 30 m, the mean of the ADEs increases by approximately 2 orders of magnitude at 10^4 a and by a factor of 4 at 10^5 a.

- For an assumed waste exclusion distance of about 200 m, the mean of the ADE would be zero at all times up to 10^5 a.

Finally, we also examined the effect of small variations in the length of the waste exclusion distance. For the reference disposal system, the minimum waste exclusion distance is about 50 m; we actually use a more precise value, 46.5 m, based on engineering drawings. We examined two other cases, where this more precise value is 45.7 and 47.5 m, or about 2% smaller and larger respectively. (Unlike other variations described here, these two cases did not involve modification of the network of segments.) The results, from sets of 500 simulations, show that

- There is a large change in the mean ADE for times up to 10^4 a. The 2% smaller waste exclusion distance leads to a 40% increase in the mean ADE, whereas the 2% larger distance leads to a 30% decrease.

- The effects are smaller for times up to 10^5 a. Both the larger and smaller waste exclusion distance change the mean ADE by only about 7%.

These results again show that the length of the waste exclusion distance is more important at early times and less important once releases do not change rapidly with time.

E.8.9 CASE 8 - VAULT ROOMS ABOVE LD1

The definition of the reference disposal system specifies a waste exclusion distance of about 50 m of sparsely fractured rock with no vault rooms located above fracture zone LD1 (Section 6.2 in the main text). Case 8 examines a variation in which we assume some vault rooms are added above LD1. It is modelled by changing

- The dimensions of the vault, which are extended by adding some vault rooms above LD1, so that the vault disposal area increases by about 7%. Some new network segments are required, as illustrated in Figure E-49, to connect the new vault rooms with LD1. The waste exclusion distance is maintained at about 50 m on both sides of LD1.

- The total inventory of the nuclear fuel waste increases by about 7%, taking account of the additional vault disposal rooms.

As for Case 7, this case is here considered to be a potential design constraint, but it may also have broader implications as a site feature related to the frequency of fractures and the groundwater velocities in the rock near a potential disposal vault.

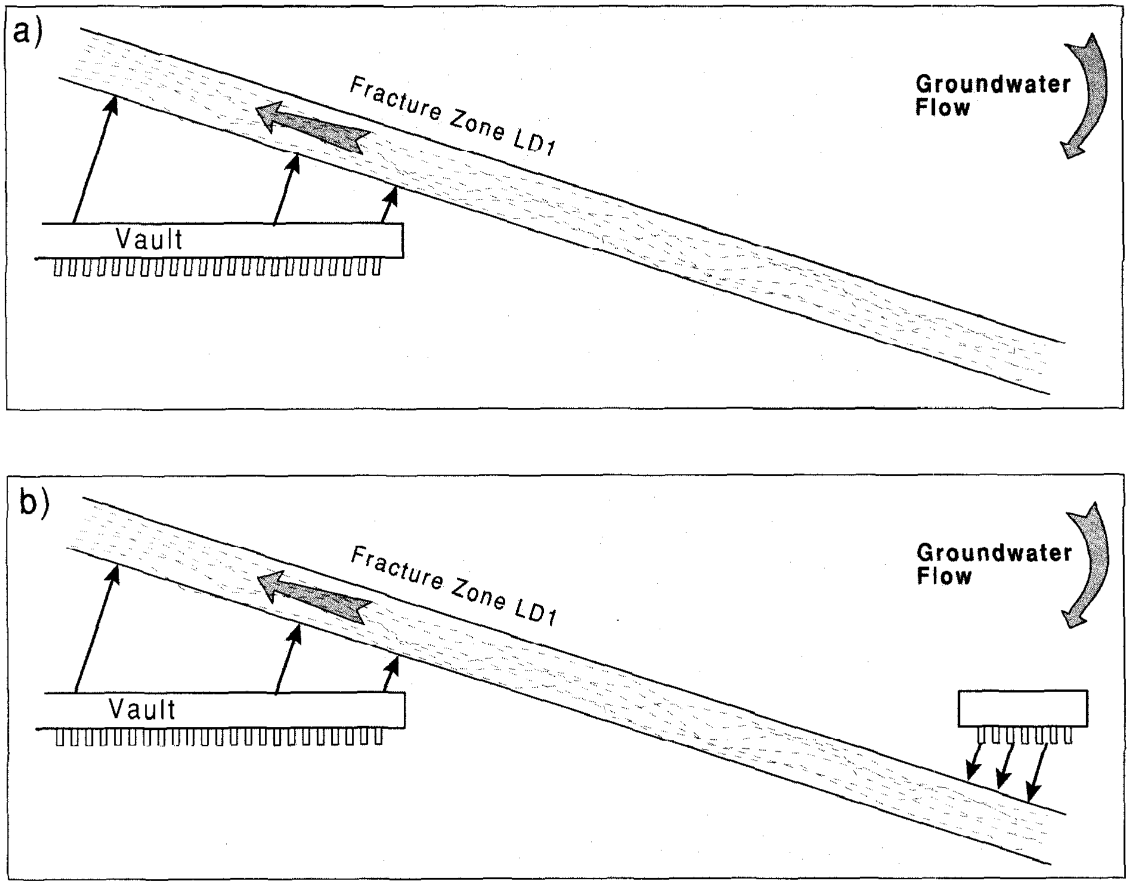


FIGURE E-49: Illustration of the Network of Segments Required for Case 8.

Both parts of this figure are cross sections through the vault, illustrating the location of fracture zone LD1 and some of the geosphere segments (shown as arrows) connecting the vault to LD1. The segments in Part (a) are used in the simulations for the reference disposal system. The segments in Part (b) are used in the simulations for Case 8 and include additional segments from the vault rooms above LD1. Groundwater flow is generally downwards in the rock above LD1, extremely small in the rock below LD1, and upwards along LD1.

Table 6-16 in the main text shows that the addition of vault rooms above LD1 leads to significantly larger ADEs at 10^4 and 10^5 a. These results can be attributed to three effects:

- The backfill is always between the buffer and LD1 for the rooms below LD1. Therefore, all contaminants from vault rooms below LD1 travel through both the buffer and the backfill (Garisto and LeNeveu 1991). On the other hand, the backfill does not lie between the buffer and LD1 for the vault rooms above LD1; for these rooms we assume that the backfill is not in the transport path and that all contaminants travel only through the buffer (Section 5.2 in the main text). Thus the introduction of rooms above LD1 leads to larger ADEs because we assume the backfill barrier is avoided for these rooms.

- Groundwater velocities toward LD1 and within the waste exclusion distance are more than 10 times faster in the rock above LD1, compared with the rock below LD1. These differences have the result that both diffusion and transport in moving groundwater are important in transporting contaminants from the vault rooms above LD1, but only diffusion is important from the vault rooms below LD1. That is, the additional rooms above LD1 leads to larger ADEs because of the increased contaminant transport from these additional rooms to LD1.

- The additional rooms above LD1 contain an increased inventory of about 7%. The increased inventory by itself has a relatively small effect.

The ADEs from ^{14}C and ^{99}Tc at 10^5 a are increased more than those from ^{129}I (Table 6-17 in the main text and Figures E-39 to E-41). The ADE from ^{14}C is affected, in addition to the three factors above, by radioactive decay; that is, the more rapid transport brings ^{14}C to the surface earlier, allowing less time for radioactive decay to reduce the amounts of ^{14}C. The half-lives of the other two nuclides are too long for decay to have much effect. The ADE from ^{99}Tc is strongly affected by the presence or absence of the backfill barrier because ^{99}Tc is sorbed on the backfill.

Figure E-50 shows a pairwise comparison of each of the 500 simulations from this case with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At both 10^4 a and 10^5 a, all the simulations are affected by the extra rooms above LD1 and show significant increases in the ADEs.

An auxiliary study examined a vault layout with and without rooms above LD1, and where the waste exclusion distance on both sides of LD1 was increased to about 70 m. Compared with Case 7, the additional size of the waste exclusion distance should reduce the ADEs, whereas the rooms above LD1 should increase the ADEs. The net effect is an increase in the ADEs, by factors of about 200 at 10^4 a and 40 at 10^5 a.

The results of Case 8 (and Case 7) are sensitive to the detailed characteristics of the site of the reference disposal system.

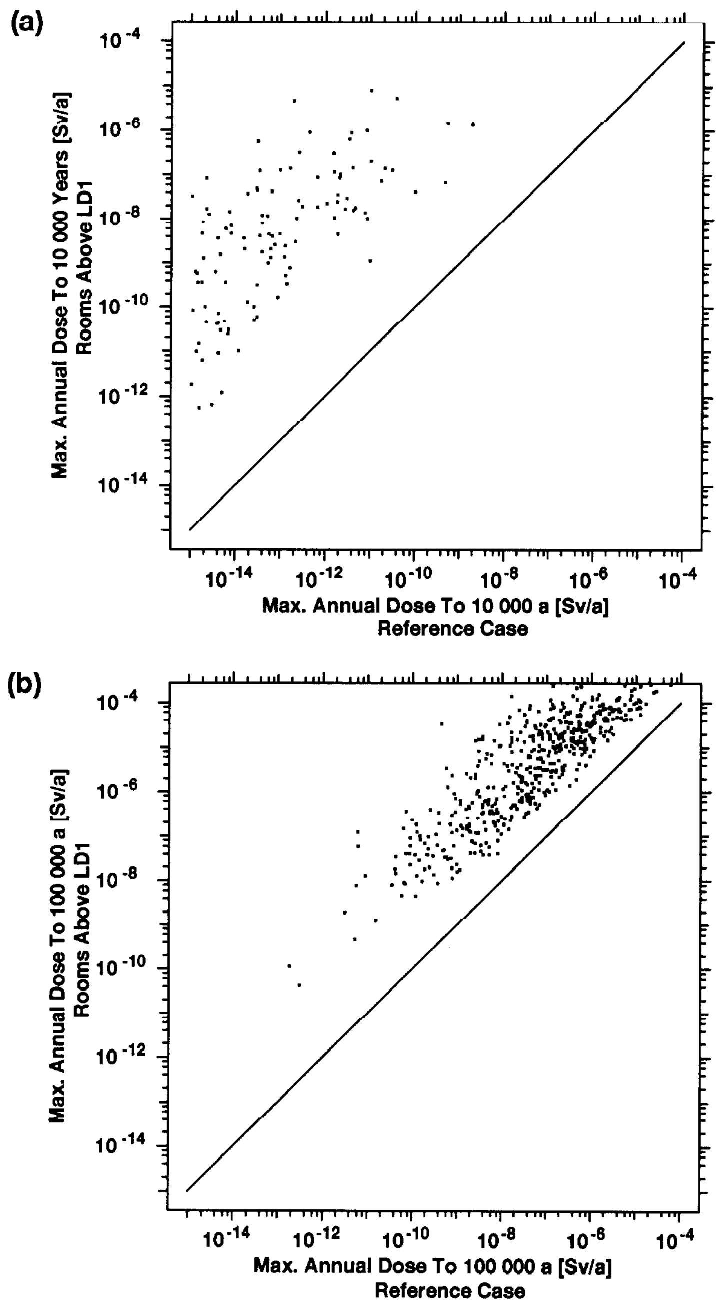


FIGURE E-50: Effect of Vault Rooms on Both Sides of LD1.

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical, except for the presence or absence of vault rooms above and to the right of fracture zone LD1. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system, with no vault rooms above LD1. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations assuming vault rooms are on both sides of LD1. Points falling on the diagonal line indicate pairs of simulations with identical results. Both sets of simulations use a waste exclusion distance of about 50 m.
The results indicate that the presence of rooms above LD1 lead to large increases in maximum ADEs.

E.8.10 CASE 9 - WELL NOT IN PLUME

The reference disposal system assumes that, in about 50% of all simulations, there is a well located above, and drawing water from, the centre of the plume of contaminated water travelling along fracture zone LD1 (Davison et al. 1994, Davis et al. 1993). In Case 9, we assume that the source of water used by members of the critical group is always the lake (or, equivalently, that their well water is no more contaminated than the water in the nearby lake). This change is not consistent consistent with current information at the site of the hypothetical vault in the WRA.

The results in Table 6-16 in the main text show that the means of the ADEs are reduced by a factor of 7 at 10^4 a and 5 at 10^5 a, principally because of the importance of the well in drawing water directly from the contaminant plume in the reference disposal system. In Case 9

- Drinking water for the critical group always comes from lake water, which generally has lower concentrations of contaminants than well water;

- Irrigation of the garden (if it is practised) also involves lake water; and

- The transport path for contaminants through the geosphere always includes migration through the upper rock zone and through the overburden and compacted lake sediment layers, which further delays releases and reduces the ADEs. Technetium is particularly affected (Table 6-17 in the main text and Figure E-41) because it is sorbed onto overburden and lake sediment. Carbon-14 is also affected because it is sorbed by the calcite present in the upper rock zone, and its relatively short half-life means less ^{14}C discharges to the biosphere.

Figure E-51 shows a pairwise comparison of each of the 500 simulations from this case with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At both 10^4 a and 10^5 a, about 250 pairs of simulations are unaffected because both use lake water as the source of water for the critical group. In the remaining 250 pairs simulations, the ADEs are reduced by up to 2 orders of magnitude when lake water is used instead of well water. The overall effect of this site feature on the mean of the ADEs is less than 1 order of magnitude because some of the simulations with largest ADEs involve the use of lake water.

E.8.11 CASES 10 AND 11 - THICKER SEDIMENT AND OVERBURDEN

In the reference disposal system, the average thickness of the compacted lake sediment is 4.7 m (Davis et al. 1993), and the average thickness of the overburden is 4.6 m (Davison et al. 1994). For cases 10 and 11 we truncate the PDFs used in the reference disposal system for these parameters to eliminate the smaller values:

- In Case 10, the minimum thickness of the compacted lake sediment is assumed to be 10 m, and the average thickness is increased to 13.0 m; and

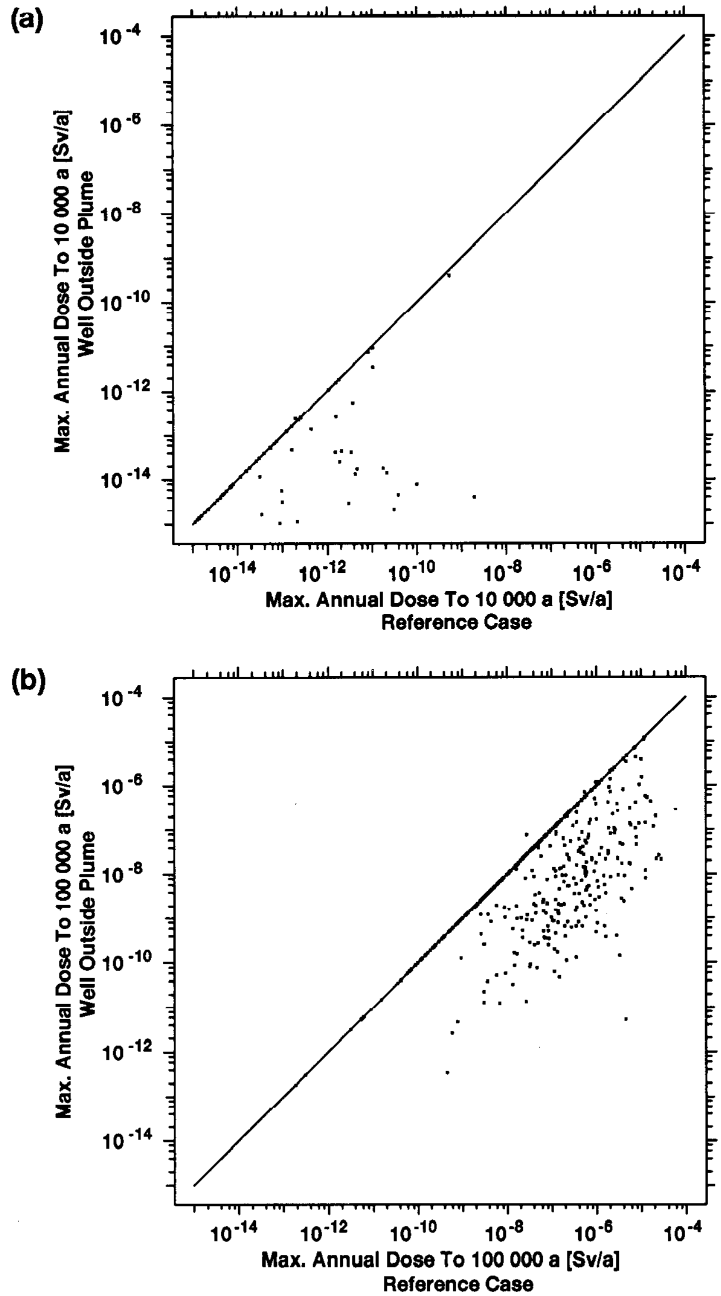


FIGURE E-51: Effect of the Use of Lake Water Only

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical, except for the source of domestic water used by the critical group. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system, in which the source of water is the well in about 250 simulations and the lake in about 250 simulations. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations in which the assumed source of water is always the lake. Identical results should be obtained for about 250 simulations where the source of water is the lake in both sets of simulations.

The maximum ADEs are much smaller for many simulations when only the lake is available as the source of water.

- In Case 11, the minimum thickness of overburden is assumed to be 20 m, such that its average thickness is increased to 21.2 m.

In both cases, the assumed increase in thicknesses is not consistent with current information at the site of the hypothetical vault in the WRA. However, the ranges are compatible with thicknesses of compacted lake sediment and overburden found on the Canadian Shield.

The increased thickness can act to delay the transport of contaminants, except for those contaminants that enter the well, and thus by-pass lake sediment and overburden. The results in Table 6-16 show that increased thicknesses of compacted lake sediment and overburden have little effect on the mean of the ADEs. The effects are minor because compacted lake sediment and overburden

- are not part of important pathways affecting the critical group whenever a well is used; and

- do not substantially delay the transport of ^{129}I; for example, in the median-value simulation, the delays are only about 200 a through either barrier (Table D-3 in Appendix D).

Figure E-52 shows a pairwise comparison of each of the 500 simulations from Case 11 (thicker overburden) with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At both 10^4 a and 10^5 a, no effects are observed for about 250 simulations in which a well is present. For the remaining simulations, ADEs are reduced with the thicker overburden. A similar pattern of behaviour is observed for thicker compacted lake sediment (Case 10).

E.8.12 CASE 12 - ORGANIC SOILS

In the reference disposal system, we assume that the nearby fields contain any one of four soil types, with the most likely soil type being sandy soil (Davis et al. 1993). In Case 12, we assume the fields consist of only organic soil.

Table 6-16 shows a small increase in the mean of the ADEs. There are two main reasons for this effect:

- Case 12 also involves changes to other parameters used in the biosphere because some parameters are correlated with soil type (Section 5.6 in the main text). For example, organic soils may require greater amounts of irrigation, and hence put a greater demand on the well when well water is used for irrigation. In turn, greater demands on the well may result in greater capture of contaminants and greater accumulation of contaminants in the garden.

- An important part of the pathways affecting the critical group is ingestion of plants grown in contaminated soil. In Case 12, contaminant concentrations in soil are greater because organic soil more strongly sorbs ^{14}C, ^{129}I and ^{99}Tc. Thus the mean of the ADEs are also greater.

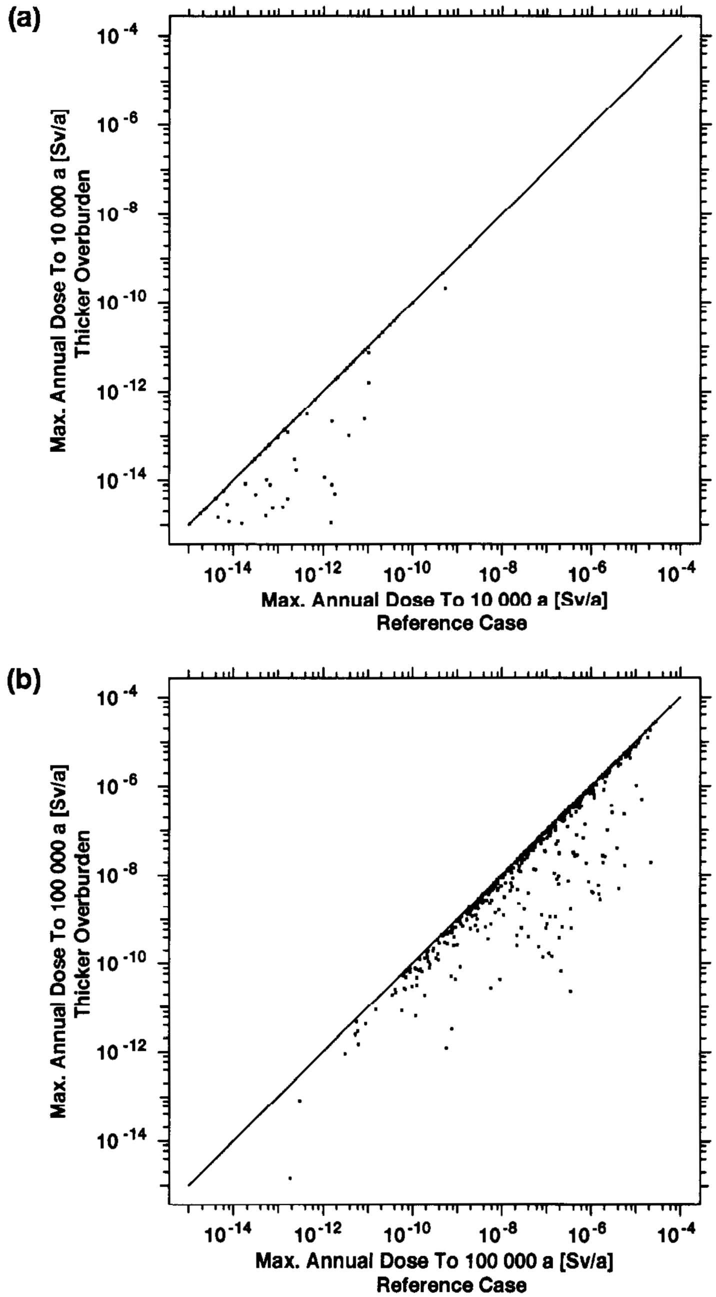


FIGURE E-52: Effect of Increased Overburden Thickness

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical except for the thickness of the overburden. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations with an assumed increase in thickness of overburden. Points falling on the diagonal line indicate pairs of simulations with identical results.

The results show that increased thicknesses of the overburden lead to smaller maximum ADEs for many simulations. Similar results are obtained for simulations with an increased thickness of compacted lake sediment.

The ADEs are more affected for ^{14}C and ^{99}Tc than for ^{129}I (Table 6-17 in the main text, Figures E-39 to E-41) because of differences in the extent of sorption of these nuclides on organic soil.

Figure E-53 shows a pairwise comparison of each of the 500 simulations from Case 12 with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At both 10^4 a and 10^5 a, the presence of organic soils gives mixed effects on the ADEs. However, the average effect is that ADEs tend to be greater with organic soils than with other types of soil.

E.8.13 CASE 13 - LARGER WATERSHED

In the reference disposal system, the average size of the watershed is 100 km^2 (Davis et al. 1993). In Case 13, we modify the PDF describing the watershed area, such that the assumed average size is 1000 km^2. This increased watershed area is not consistent with lakes near the reference disposal system.

A larger watershed area provides larger flows of water through the lake, and thus larger dilution of contaminants that have entered the lake. The results in Tables 6-16 and 6-17 in the main text show that there are only small decreases in the ADEs, primarily because the critical group is more affected by water from the well than by water from the lake.

Figure E-54 shows a pairwise comparison of each of the 500 simulations from Case 13 with the first 500 randomly sampled simulations used in the analysis of the reference disposal system. At both 10^4 a and 10^5 a, about 250 simulations involving the well are unaffected by an increased watershed area. Of the remaining 250 simulations, some show the full one-order-of-magnitude dilution effect, and others show an intermediate effect.

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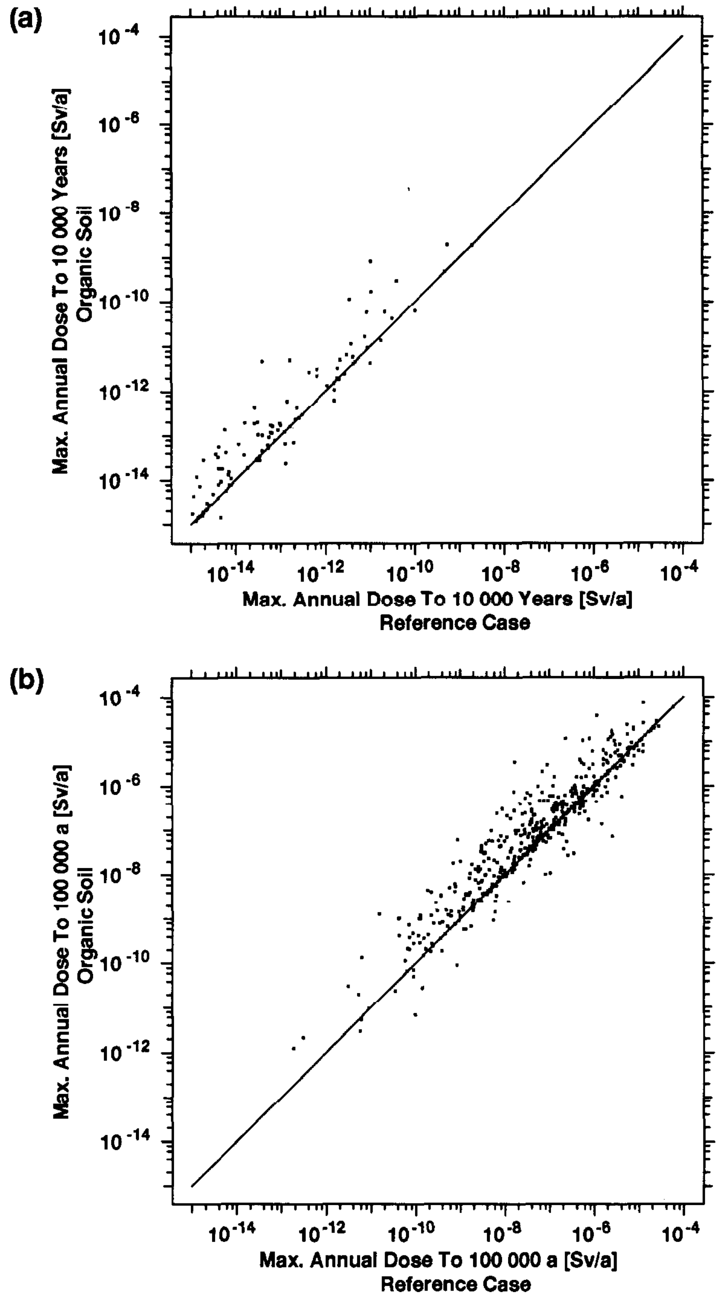

FIGURE E-53: Effect of Soil Type

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical except for the soil type in the garden (and other fields) used by the critical group. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system, in which the selected soil type is sand, loam, clay or organic in about 57%, 5%, 24% and 14% of the simulations respectively. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations where the assumed soil type is organic. Points falling on the diagonal line indicate pairs of simulations with identical results.
In most simulations, the use of organic soil leads to larger maximum ADEs.

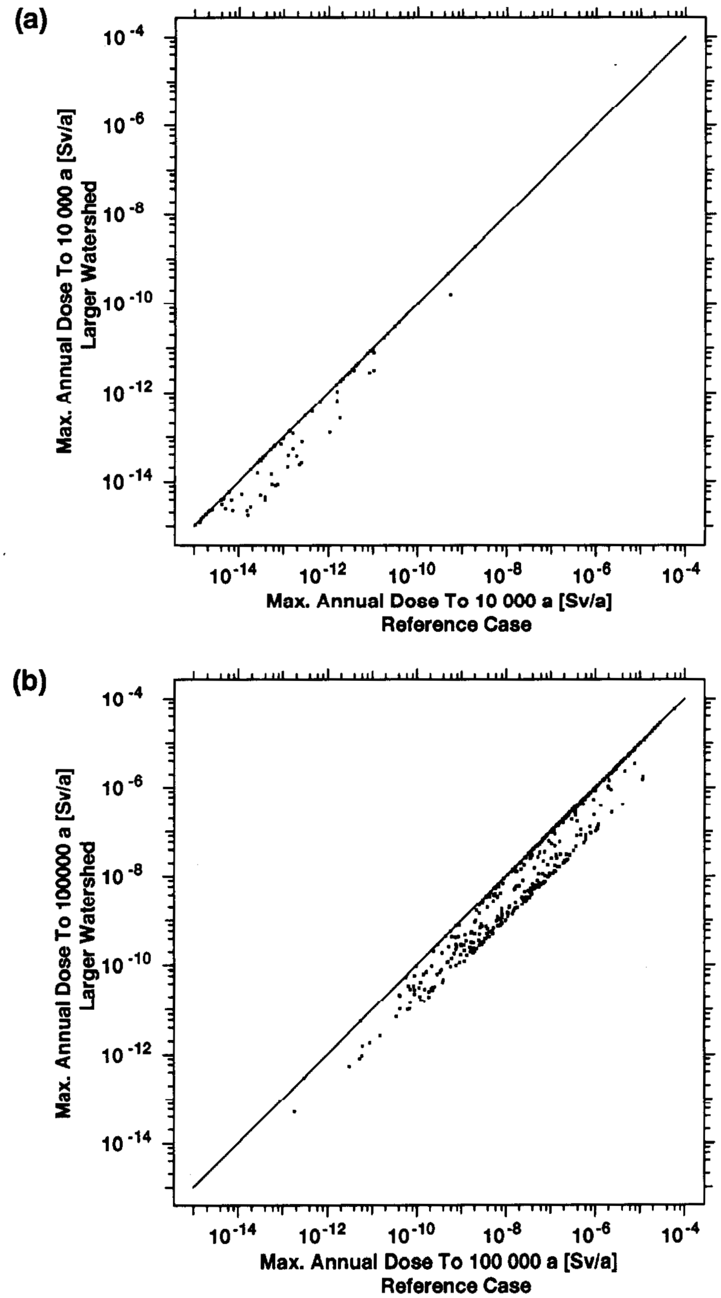

FIGURE E-54: Effect of Increased Watershed Area

These scatter plots show 500 pairs of maximum ADEs for times up to 10^4 a (part a) and up to 10^5 a (part b). Each symbol plots the results from two simulations that are identical except for the size of the watershed area feeding the lake. The horizontal axes show maximum ADEs from the reference case: the first 500 randomly sampled simulations used in the analysis of the reference disposal system. The vertical axes also show maximum ADEs but taken from 500 randomly sampled simulations with a larger assumed watershed area. Points falling on the diagonal line indicate pairs of simulations with identical results.
A larger watershed area leads to smaller maximum annual dose estimates for many simulations.

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APPENDIX F

PROBABILITIES OF OCCURRENCE OF METEORITE STRIKES AND EARTHQUAKES FOR THE REFERENCE DISPOSAL SYSTEM

CONTENTS

F.1 INTRODUCTION

Appendix F discusses two topics related to scenario analysis: the probabilities of occurrence of meteorite strikes and earthquakes. We examine these two rare events and provide estimates of their probabilities of occurrence for cases where they occur close enough to the reference disposal vault to cause a significant disruption to the integrity of the disposal system.

F.2 PROBABILITY OF OCCURRENCE OF METEORITE STRIKES

Grieve and Robertson (1984) note that about 10^5 kg of meteoroids (or interplanetary material) enter the Earth's atmosphere every day, but most of them burn up or disintegrate in the atmosphere. Meteorites are those meteoroids that reach the Earth's surface, and smaller meteorites are more common than larger ones. Meteorites have impact velocities of the order of 20 to 25 km/s and release large quantities of energy. For example, "the energy released in forming the relatively small 3.8-km Brent crater, Ontario is estimated at . . . the same order of magnitude as the annual output of seismic energy by the earth" (Grieve and Robertson 1984). The effects of such impacts include penetration of the target rocks to a depth of several radii of the meteorite and the formation of a meteorite crater that damages the underlying rock.

In discussing this damage, Grieve and Robertson (1984) distinguish between simple and complex craters: simple craters, with diameters less than 4 km, have deeper effects relative to their diameter than do complex craters whose diameters are greater than 4 km. Simple craters tend to exhibit the bowl-like cross section shown in Figure F-1, whereas complex craters show a structure with (more) pronounced uplift in the centre.

Grieve and Robertson (1984) describe the effects of a meteorite crater on five different zones of rock in the impact area.

- Rock at the point of impact is excavated and ejected. The depth of excavation (from the original land surface) is about 10% of the crater diameter for simple craters and up to 6.5% for complex craters.

- Underlying rock is moved and redistributed within the confines of the crater. This rock is highly shocked and impact-melted and extends to a depth, from the original land surface, of about 14% of the crater diameter for simple craters but only 9% for complex craters. As indicated in Figure F-1, this depth lies somewhat off-centre from the point of impact.

- At greater depths, rock is shocked and compressed, and displaced but not redistributed. For simple craters, this zone extends downwards to about 42% of the crater diameter. For complex craters, the depth is about 25% of the crater diameter.

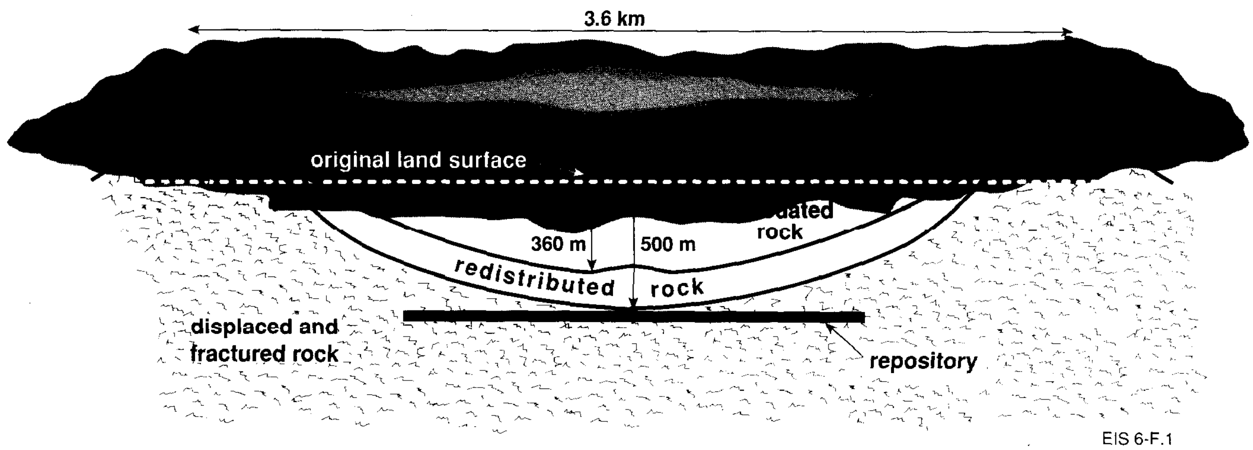

FIGURE F-1: Effects of a Meteorite Strike

In the analysis described herein, we assume that a meteorite strikes the surface of the Earth directly above the disposal vault. We examine the case where the meteorite is sufficiently large that it leaves a 3.6-km diameter crater and completely disrupts the rock above the disposal vault. The maximum depth of excavated rock is about 360 m, and a further 140 m of rock is redistributed. Rock below 500 m is not redistributed but may be shocked, compressed and fractured.

- A larger zone of fractured rock surrounds the impact site. The diameter of the zone of fractured rock is about 1.5 times the diameter of a simple crater, and 2.7 times the diameter of a complex crater. For both simple and complex craters, the estimated depth of fracturing is about 76% of the crater diameter.

- Seismic energy from the impact may affect rock far beyond the immediate area of the crater. The effects would be greater in rock that is highly stressed.

We are concerned here with the probability of occurrence of a meteorite that strikes near the disposal site and that disrupts the integrity of the disposal system. We examine the specific case in which a large meteorite creates an impact crater about 3.6 km in diameter (Figure F-1). Based on the above discussion, this crater diameter is sufficiently large that

- The depth of excavation would be about 360 m. That is, about 1.9×10^9 m^3 of rock from as deep as 360 m would be excavated and ejected from the site of the impact.

- Rock to a depth of about 500 m would be moved and redistributed throughout the crater. This volume of rock, about 7.5×10^8 m^3, would be dispersed into the lens-like shape shown, with a maximum depth of about 140 m from the interior surface of the crater.

- There is a larger zone of underlying rock that would be displaced (shocked and compressed) and fractured. The extent of fracturing is estimated to extend to a diameter of 5.4 km at the surface and to a depth of about 2.7 km.

Figure F-1 also shows the presumed impact site, located immediately above the geometric centre of the disposal vault. It follows that the depth of the redistributed rock would just extend to the horizon of the vault, for a disposal vault at a depth of 500 m (the nominal minimum depth in the concept for disposal of Canada's nuclear fuel waste).

An estimate of the probability of occurrence of a crater like that in Figure F-1 can be made using the relationship from Grieve and Robertson (1984):

$$N = 2.0 \times 10^{-12} D^{-2}$$

where D is the crater diameter in kilometres, and N is an estimate of the frequency of occurrence, per year and per square kilometre, of a crater of diameter D or larger. For a crater diameter of 3.6 km or greater, N is equal to 1.5×10^{-13} km^{-2} a^{-1}.

To estimate an annual probability of occurrence of a meteorite strike, we require a measure of the areal extent affected by the impact. A crater 3.6 km in diameter would affect an area approximately equal to the area of the disposal vault. A larger crater would have a deeper and more widespread zone of redistributed rock and could intersect the disposal vault even if the impact site were some distance away from the vault. Thus larger craters are less likely to occur, but they are associated with a larger area where rock at a depth of 500 m is redistributed but not ejected. Grieve and Robertson (1984) describe a procedure to take into account the areal extent. Using their procedure, we estimate a probability of about 1.4×10^{-11}/a that a meteorite would produce a zone of redistributed rock that intersects the disposal vault.

Thus our analysis shows that the probability of occurrence is very small for a specific case in which a meteorite causes redistribution of rock at a depth of 500 m. Slightly larger (smaller) probabilities would apply to meteorites that would produce less (more) damage to the disposal vault. In estimating these probabilities, we have not taken into consideration variations in probability of meteorite impacts with latitude and time. We expect these variations would be relatively small. Thus similar probabilities of occurrence for meteorite impacts would apply to a disposal vault at 500 m depth at any terrestrial location.

F.3 PROBABILITY OF OCCURRENCE OF EARTHQUAKES

Earthquakes are a series of suddenly generated elastic waves in the Earth, occurring to depths of about 700 km (Lapedes 1978). They are caused by the sudden release of energy in the earth when stresses in the rock have grown greater than the rock strength. The stress is relieved when the rock breaks, and the sudden movement generates elastic waves.

Earthquakes are generally associated with the extremely slow movement of material in the mantle, causing the movement of parts of the earth's crust, called plates. The process is called plate tectonics. A plate is an independent segment of the crust and solid upper mantle of the earth that moves horizontally relative to other segments and interacts with them along its margins. Where breaks (rifts) occur in the crust, new plate material is created as molten material from the lower mantle comes to surface and solidifies into rock as it cools. The new crust that is formed spreads away from the rift as the plates diverge. Movement of the plates induces the gradual drifting of continents on the earth's surface and could generate faulting in the interior regions of continents, including the Canadian Shield.

Johnston and Kanter (1990) show that earthquakes are much less frequent at rifted portions of the crust than at plate boundaries, and even more infrequent at unrifted portions of the stable crust. Their data shows a frequency of about $6 \times 10^{-11}/km^2/a$ for earthquakes of magnitude greater than 6 on unrifted portions of stable shields. (Earthquake magnitudes are frequently expressed using the logarithmic Richter scale, with recorded values as high as 8.9 (Strahler 1981). An earthquake of magnitude 4 can cause local damage, whereas one of magnitude 6 can be destructive in a limited area.)

The Canadian Shield is the least seismically active portion of the North American plate and one of the least seismically active regions in the world. Although infrequent but detectable earthquakes occur throughout the Shield, most with magnitude greater than 4 tend to occur along the shield margins or along very large faults and the regions of most recent rifting

(Adams and Basham 1991). Most of the large earthquakes in eastern Canada have been be related to the location of ancient rifts in the North American plate (Adams and Basham 1991). In Ontario, earthquakes are concentrated near the Ottawa Valley (an old rift) and along the Kapuskasing structural zone (a 400-km long feature believed to be a deep crustal thrust fault (Percival and Card 1985)).

Because earthquakes tend to occur in zones that have exhibited seismic activity in the past and because potential effects of an earthquake would depend on the the characteristics of a particular disposal site, we examine probabilities for a particular site: that of the (hypothetical) reference disposal system. We are concerned here with the probability of occurrence of an earthquake sufficiently near the disposal site that it disrupts the integrity of the disposal system.

The disposal system could be affected if it were near enough to the focus (or centre) of a large earthquake. The potential significant effects are disruption of the engineered barriers and disruption of the rock surrounding the disposal vault. Damage could result from

- the formation of a new fault,
- the movement of an existing fault with possible extension of branching faults or splays into the surrounding rock, and
- shaking of the disposal vault and its contents caused by the elastic waves.

If damage occurred, it could lead to new or altered pathways for movement of contaminants that are in the disposal vault at the time of the earthquake or that have been released from the disposal vault prior to the earthquake. Damage within the vault could decrease the effectiveness of containers, buffer and backfill, and increase the rate of release of contaminants from the disposal vault. We consider only these adverse effects. Nevertheless, it is possible that an earthquake could actually improve the performance of the disposal system. For instance, a new fault could change hydraulic heads so that groundwater flow near and through the disposal vault decreases, or the extension of an existing fault could draw greater quantities of uncontaminated water so that contaminant concentrations are decreased in that fault.

We examine below the probability of formation of new faults, the probability of extending existing faults, and the probability of damaging the vault and its contents.

From our studies at the WRA, we believe that the formation of a new fault nearby would not be a credible event over the next 10^4 a.

- The reference disposal system is located on an unrifted portion of the Canadian Shield. Our studies of the fracture zones at the WRA indicate they were formed during the cooling phase of the Lac du Bonnet Batholith, approximately two billion years before present (Davison et al. 1994a). In addition, studies at the Underground Research Laboratory (URL) in the WRA suggest that the existing fracture zones are inactive, and they have not experienced recurrent periodic movement within the last 10^6 a (Davison et al. 1994a).

If an earthquake did occur near the reference disposal system, it is more likely that an existing fault would be extended than a new fault would be formed, in part because existing faults are weaker than either moderately fractured or sparsely fractured rock (Davison et al. 1994a). However, we believe that the conditions in the vicinity of the reference disposal system are such that the probability is less than 10^{-8}/a that an existing fault would be extended sufficiently to be of concern for at least the next 10^4 a.

- As noted above, our studies at the URL indicate that existing faults and fracture zones are inactive. The greatest extent of splays and secondary fractures associated with the most extensive fracture zone at the URL is only about 100 m, and it is likely that any these extensions occurred long ago, during times of plate collisions and following the retreat of glaciers (Davison et al. 1994a).

  Atkinson and McGuire (1993) estimated the probability that fractures would extend to reach a disposal vault as a result of a nearby earthquake. Their estimates indicate this probability is less than 10^{-8}/a, provided the vault is not near an active fault. Specifically, the vault should not be within 1 km of a 2-km-long active fault, or within 200 m of a 500-m-long active fault, or within 50 m of any other active fault. We believe these conditions are met for the reference disposal system. For example, the nearest fracture zone (thought to be inactive) is about 50 m from any room in the reference disposal vault (see the fracture zone labelled LD1 in Figures 5-5 to 5-7 and 5-13).

Finally, the probability of damage to the disposal vault by an earthquake depends on a number of factors, including the proximity of the vault to the focus of the earthquake, rock strength, and the design and orientation of the vault. Because the reference disposal system is located in an area that is seismically inactive, we believe that the probability is less than 10^{-8}/a that there would be significant damage to excavated disposal vault or its contents for at least the next 10^4 a.

- Dowding and Rozen (1978) have surveyed the effects of earthquakes on underground openings. They report that peak ground accelerations of less than 20% of the acceleration resulting from gravity (0.2 g) have produced no detectable damage, and accelerations up to 0.5 g produced only minor damage to excavation surfaces. Studies by Ates et al. (1994) on the potential effects of earthquakes on a closed disposal vault show that earthquakes of magnitude 6 would produce accelerations less than 0.5 g when the earthquake focus is about 10 km from a disposal vault. We expect that much larger accelerations would be necessary to cause significant damage to a closed excavation because of the support offered by the buffer, backfill and seal materials (Ates et al. 1994). From these studies and from the frequency data of

> 6×10^{-11} earthquakes of magnitude 6 or greater per square kilometre from Johnston and Kanter (1990), the associated probability of occurrence would be about 10^{-8}/a or less of an earthquake sufficiently strong to damage the vault and its contents.

We conclude there is a small probability (less than 10^{-8}/a) that an earthquake of sufficient magnitude would occur near enough the reference disposal system to cause significant damage. More generally, our studies indicate that it is very probable the integrity of any closed vault and its surrounding plutonic rock mass would be maintained for the next 10^4 a if the disposal vault were sited far from regions of clustering of current earthquake activity, far from major regional fault zones on the Shield and far from ancient rifts. These considerations would contribute to the site selection process (Davison et al. 1994b).

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APPENDIX G

GLOSSARY

<u>absorbed dose (D)</u>: The quantity of energy transferred from radiation to a mass of a substance. The SI unit of measurement of absorbed dose is the gray (Gy). See dose equivalent.

<u>actinide</u>: An element with an atomic number from 89 (actinium) to 103 (lawrencium). All actinides are radioactive. Examples are thorium, uranium and plutonium.

<u>activity</u>: The number of nuclear disintegrations occurring in a given quantity of material per unit time. The SI unit of activity is the becquerel (Bq); 1 Bq = 1 disintegration per second.

<u>acute dose</u>: A high dose of radiation received in a very short time. It is expressed in sievert (Sv). Radiation sickness or other effects could occur if dose rates are sufficiently high. Compare with chronic dose.

<u>ADE</u>: An abbreviation for annual dose estimate. More precisely, it is an estimate of the 50-year committed effective dose equivalent from internal exposure plus the effective dose equivalent from external exposure, occurring over a year. It is the same as the annual effective dose equivalent and its units are Sv/a.

<u>adsorption</u>: Adhesion of ions, molecules or particles to the surface of solid bodies with which they come in contact. See sorption.

<u>advection</u>: 1. Transport of material or energy by a moving fluid. 2. In meteorology, the transport of an atmospheric property solely by the mass motion of the atmosphere. 3. In limnology, the vertical or horizontal transport of water, or of an aqueous property, solely by the mass motion of the fluid.

<u>AECB</u>: See Atomic Energy Control Board.

<u>alpha particle (α)</u>: The nucleus of a helium atom, consisting of two protons and two neutrons. It has a charge equal to two electrons but with the opposite (positive) sign. Alpha particles are commonly emitted from heavy radionuclides such as ^{239}Pu when they decay. These particles transfer their energy within a very short distance and are readily shielded by a piece of paper or a layer of dead human skin. See alpha radiation.

<u>alpha radiation</u>: The emission of alpha particles from the nucleus of unstable atoms. Since alpha radiation cannot penetrate the outer layer of human skin, it is not normally a radiation hazard to humans and animals, unless it is located inside the body. See alpha particle.

<u>alternative scenario</u>: As used in the postclosure assessment, alternative scenario refers to some feasible combination of factors (features, events and processes) that describes a possible but not the most probable behaviour of the disposal system in time. This combination of factors also describes a possible mechanism for the release of contaminants from their engineered containment,

followed by transport to the biosphere. In the assessment of the reference disposal system, the open-borehole scenarios and the inadvertent human intrusion scenarios are regarded as alternative scenarios, whereas the SYVAC scenarios are the most probable.

annual dose: *An abbreviation for committed effective dose equivalent. See* that term.

annual dose estimate: See ADE.

annual effective dose equivalent: the sum, over one year, of the effective dose equivalent resulting from external exposure and the 50-year committed effective dose equivalent from that year's intake of radionuclides by a member of the critical group. It is the effective exposure over one year to low doses of ionizing radiation, and takes into account different types of radiation and the potential effects on different organs (see dose equivalent and effective dose equivalent). It is frequently abbreviated as ADE in the postclosure assessment. The SI unit of measurement of annual effective dose equivalent is the sievert per year (Sv/a).

aquatic concentration ratio: The ratio of the nuclide concentration in the edible portion of fish to the concentration in water. It quantifies the transfer of a nuclide from the lake environment to fish.

associated dose limit: In the postclosure assessment, an annual dose that conforms with the AECB risk criterion. The associated dose limit is derived from the radiological risk criterion set by the AECB. For a risk limit of 10^{-6} (probability of serious health effects per year), and assuming that only one scenario contributes to the risk, the associated dose limit is the risk limit divided by the risk factor (2×10^{-2} serious health effects per sievert as specified in AECB Regulatory Document R-104). Thus the associated dose limit is 5×10^{-5} Sv/a or 50 μSv/a. It is about 2% of the annual dose that residents of the Canadian Shield receive from natural sources of radiation. Compare with conditional risk.

atom: The smallest particle of an element that maintains the properties of the element and can enter into chemical combination. Atoms are composed of protons, neutrons and electrons. The protons and neutrons adhere to each other in a dense nucleus, surrounded by a cloud of electrons. Electrically neutral atoms have an equal number of protons and electrons. Different isotopes of a given element are atoms with the same number of protons but a different numbers of neutrons. Ions are atoms that have gained or lost electrons and are, therefore, electrically charged. See also nuclide and radionuclide.

Atomic Energy Control Board (AECB): The Canadian federal regulatory agency that has jurisdiction over nuclear facilities and nuclear materials, and exerts regulatory control through a comprehensive licensing system. Established in 1946, the Board's mandate is "to ensure that the use of nuclear energy in Canada does not pose undue risk to health, safety, security and the environment".

Through its licensing and inspection systems, the AECB provides control and supervision of the development, application and use of atomic energy in Canada, and participates on behalf of Canada in international measures of control.

backfill: In a disposal vault, the material used to refill excavated portions in disposal rooms, shafts and tunnels after the waste packages and buffer have been emplaced. In the CNFWMP, the backfills being considered are: a mixture of glacial lake clay and crushed granite from the vault excavation and a mixture of sodium bentonite clay and silica sand.

background radiation: Radiation doses received by the public from sources other than nuclear facilities. These sources can be broadly categorized as: 1. naturally occurring radiation (see natural background radiation), 2. fallout from nuclear weapons testing, 3. radionuclides present in the environment because of technological processes other than the operations of nuclear facilities, 4. irradiation from consumer products and services and, 5. medical diagnostic and therapeutic radiological processes.

batholith: A large mass of intrusive igneous rock, most of which consolidated at a considerable depth below the surface of the earth. Similar to a pluton except that it is much larger.

becquerel (Bq): The SI unit of radioactivity for measuring the rate of decay of a radioactive substance. It is equivalent to the disintegration of one radioactive nucleus per second.

bentonite: Absorptive colloidal formed by the chemical alteration of volcanic ash. It is composed mainly of montmorillonite and related minerals in the smectite group. Sodium-rich bentonite has a particular attraction for water and swells when wet. It is being considered as a major component of the buffer material used in a disposal vault.

beta particle (β): A free electron or positron emitted by a radionuclide during radioactive decay. Beta particles can penetrate biological tissue to a depth of 1 to 2 cm, or aluminum to a few mm. It can be an internal and/or external hazard to humans and other biota. See also beta radiation.

beta radiation: The emission of electrons or positrons (positively charged "electrons") by the nucleus of an unstable atom. See also beta particle.

biosphere model: The biosphere model describes the transport of contaminants within the local surface water, soil, atmosphere and the food-chain to man, including the resultant health impact of contaminants on members of the critical group. In the SYVAC3-CC3 computer model, the disposal system is modelled using a system model that contains models for the vault, geosphere and biosphere. These models were introduced to simplify the development of mathematical models of complex processes. See BIOTRAC.

BIOTRAC: A computer code written at AECL Research, Whiteshell Laboratories, to model BIOsphere TRansport And Consequences associated with nuclear fuel waste disposal. It was written to serve as the biosphere model in SYVAC3-CC3 and is used in the postclosure assessment of the reference disposal system.

buffer: In the CNFWMP, a highly impermeable material that would be placed around the waste containers in a disposal vault. The primary purpose of this material is to serve as an additional barrier by retarding the movement of water, such that contaminant movement away from the containers would be dominated by diffusion. It would also affect the rates of container corrosion, fuel dissolution, and radionuclide migration. In the postclosure assessment study, the buffer material is a compacted sand-bentonite mixture.

buffer anion correlation parameter: A parameter that correlates the values of the buffer diffusion coefficient and the buffer capacity factor for all contaminants in the vault that are expected to form anionic species in groundwater.

buffer capacity factor: The ratio of the total amount of a species per unit volume of porous medium to the amount of the species in solution per unit volume of the same medium.

buffer diffusion coefficient: See diffusion coefficient.

Canadian Nuclear Fuel Waste Management Program (CNFWMP): A program of research and development on radioactive waste management established in a 1978 Joint Statement by the Federal Government and the Government of Ontario. The aim is to develop and assess the concept of disposing of nuclear fuel waste in the plutonic rock of the Canadian Shield. AECL is responsible for verifying the safety of this disposal method. Ontario Hydro is responsible for developing and demonstrating nuclear fuel waste storage technology and for transportation of this waste from reactor sites. A second Joint statement in 1981 imposed the restriction that the concept must be assessed, reviewed and accepted before site-specific activities would be undertaken.

CANDU: CANada Deuterium Uranium, the name of the Canadian-designed reactor that uses natural uranium fuel and is moderated by heavy water. CANDU is a registered trademark of Atomic Energy of Canada Limited.

case: In the postclosure assessment, a set of SYVAC simulations for one waste disposal system, one set of models, one set of nuclides and one set of parameters and parameter probability density functions. Data from a case are usually analyzed together statistically to generate estimates of mean annual dose, risk, etc. These simulations represent all factors defining the SYVAC scenarios.

chronic dose: A dose of radiation received at a low rate over a long period of time. It is expressed in sievert (Sv). There would be no immediate effects such as radiation sickness, but other serious health effects (such as radiation-induced cancer) may occur in the future. In the postclosure assessment, we assume a dose rate of 1 Sv/a would lead to serious health effects because estimated doses attributed to a nuclear waste disposal facility are expected to be small and to persist for long periods of time. Compare with acute dose.

CNFWMP: See Canadian Nuclear Fuel Waste Management Program.

collective dose: The total dose for a population, usually based on the committed effective dose equivalent and effective dose equivalent. The collective dose can be calculated by multiplying the average dose for the exposed population by the number of people in the population. The unit used is person-Sv. See also radiological dose, effective dose equivalent and committed effective dose equivalent.

colloid: A dispersion of a solid, liquid or gas in another solid, liquid or gas. A colloid has characteristic dimensions of 10^{-9} to 10^{-6} m.

committed effective dose equivalent: The summation over time of either the dose equivalent rate or the effective dose equivalent rate over some specified time, usually 50 years for an individual. It is the dose a person would receive over a lifetime, measured in Sv/a, after an internal intake of a radionuclide. For external exposure there is no intake of radionuclides and, hence, no commitment. However, in such cases, the effective dose equivalent in Sv/a can be added to the committed effective dose equivalent from internal exposure to assess the combined exposure. See also radiological dose, dose equivalent, effective dose equivalent and risk factor.

compartment model: A mathematical description of transfers between regions (such as an a lake and its watershed, or a soil zone), for which it is assumed that the properties of interest are homogeneous in each region. This assumption may arise because relevant processes occurring within the region occur uniformly and relatively quickly. Compartment models are used within SYVAC3-CC3 to describe the concentration or mass of contaminants in different parts of the vault and biosphere. In the compacted lake sediment zone of the biosphere, for instance, it is assumed that contaminants enter and exit the sediment in groundwater, and that resulting contaminant concentrations in sediment may be estimated using selected values for controlling parameters such as the amount of diluting water present and the degree of sorption of contaminants onto sediment particles.

concentration ratio (CR): The concentration of a radionuclide present in an organism, an organ, or a tissue, divided by the concentration of that radionuclide in the surrounding medium. For example, *BIOTRAC uses a plant/soil concentration ratio (which is dimensionless)* in its food-chain and dose model.

conditional risk: In the postclosure assessment, the product of the estimated annual dose for a single scenario and the risk factor (2×10^{-2} serious health effects per sievert as specified in AECB Regulatory Document R-104). This product equals the total radiological risk if the scenario were the only one requiring quantitative evaluation in the assessment. Compare with associated dose limit.

connected porosity: The porosity of voids connected together into a network that will allow fluid flow. It excludes isolated pores.

consequence: 1. The results or effects of an event, decision or action. For the postclosure assessment in the EIS, the consequence of most concern is the mean annual dose received by an individual in the critical group at selected times. Other consequences are concerned with potential chemical toxicity impacts. 2. In the SYVAC3-CC3 computer code, calculated variables that describe some aspect of the waste disposal system. They include variables such as annual dose, maximum annual dose and container failure rate.

contaminant: As used in the postclosure assessment, material from the disposal vault that may lead to toxic effects on members of the critical group or other biota. Contaminants include both radioactive and nonradioactive nuclides.

container: See disposal container.

continuous random variable: A random variable X with a continuous cumulative distribution function F(x) and a probability density function f(x)=F′(x) (the derivative of F(x)) that is continuous except possibly at a finite number of points. In essence a continuous random variable has an infinitessimal probability of taking any specific value, but it has a finite probability of falling within certain intervals.

convective transport, contaminant: The movement of particulate or dissolved contaminants by mass movement of the medium (such as groundwater) in which they are suspended or dissolved.

convolution: One of the mathematical operations used in SYVAC3-CC3 to estimate the flow of radionuclides through a barrier. Two pieces of information are required: *the time-dependent input of radio*nuclides and a description of how the barrier responds to a standard input (the response function). The result of a convolution is the flow of radionuclides out of the barrier. In more general terms, we use a mathematical procedure involving Green's functions to solve sets of differential equations.

critical group: For a given radiation source, a group (hypothetical or otherwise) composed of members of the public whose exposure is reasonably homogeneous and who are typical of individuals expected to receive the highest effective dose equivalent or dose equivalent from the source. For the postclosure assessment, the critical group is assumed to be a hypothetical series of self-sufficient communities that live their entire life at, and obtains all their food, clothing, home furnishings, heating fuel and building materials from, the locality where there is the largest radiological impact due to contaminant release from a hypothetical disposal vault.

cumulative distribution function: For a random variable X, a function F(x) equal to the probability, P, that X has a value less than or equal to x; i.e. $F(x) = P(X \leq x)$; used in SYVAC to set the values of sampled parameters. It is the integral of the associated probability density function from $-\infty$ to x.

cumulative frequency distribution curve (upward and downward): In SYVAC calculations, a plot of the fraction of simulations in which the value of a variable is above (upward) or below (downward) particular values.

Darcy's law: An empirical relation typically used in the study of fluid flow through porous media such as rocks and soils. It relates the flux of a fluid through a medium to the hydraulic gradient:

$$q = K\, \underline{n} \cdot \underline{\nabla} h$$

where q is the flux, volume of fluid per unit area per unit time, of a fluid or gas through the medium ($m^3/(m^2 \cdot s)$). The quantity q is called the specific discharge or the Darcy velocity because the units of q reduce to those of a velocity (m/s).
K is the proportionality constant called the hydraulic conductivity (m/s),
$\underline{\nabla} h$ is the gradient of hydraulic head or the hydraulic gradient (-), and
$\underline{n}$ is the unit vector normal to the area across which the flux is being considered (-).

Darcy velocity: The flux of fluid through a medium (m/s). It is equivalent to specific discharge. See Darcy's law.

daughter product: A nuclide that is directly produced by the radioactive decay of a radionuclide. Also known as daughter or progeny.

DCF: See dose conversion factor.

decay: See radioactive decay.

decay constant: For a radionuclide in a particular energy state, the rate at which it undergoes radioactive decay. The SI units of measurement of the decay constant are s^{-1}. It is related to the radioactive half-life by the equation:

$$\text{decay constant} = \ln 2 \,/\, \text{half-life},$$

where ln 2 is the natural logarithm of 2, approximately equal to 0.69315.

decision variable: In the SYVAC3-CC3 models, a parameter that selects which alternative, or selects which probability density function (PDF) in a set of PDFs for a parameter, to use in a simulation. For example, decision variables are used to select among alternatives in the models such as the possible sources of domestic water used by members of the critical group (i.e., a well or a lake). See also switch.

dependent parameter: A scalar quantity or an element of a vector or array used by a model (usually a computer model) that is computed using mathematical equations and a set of input parameters. In SYVAC3-CC3, dependent parameters are calculated once per simulation; examples include the rate of failure of containers, the fraction of contaminants captured by a well and the concentration of radionuclides in soil.

deposition velocity: The radionuclide flux ($mol/(m^2 \cdot s)$) of airborne particles or gases to a specified surface (such as vegetation or soil), divided by the radionuclide concentration in the air above the surface (mol/m^3). The SI unit of measurement of deposition velocity is m/s.

depth of well: The depth below the water table of the well, measured to the top of the fracture zone used as well aquifer. The well is used as a water source of the critical group, a rural household. Shallower wells capture some water from the surface thus diluting contaminants captured from deep groundwater. Deeper wells capture only groundwater from the plume and capture it earlier allowing less time for decay.

derived constraint: A feasible restriction on a part of the disposal system determined to be effective in lowering annual doses to the critical group based on results of sensitivity analysis on simulations of the disposal system.

design constraint: A feasible restriction on a part of the disposal system, determined to be effective in lowering annual doses to the critical group, that is controlled by engineering design. For example, a design constraint might be the thickness of the walls of the container.

deterministic analysis: A technique for studying system behaviour mathematically using the laws of science and engineering, and assuming that all system parameters, events, and features are precisely defined. Compare with probabilistic analysis.

deterministic sensitivity analysis: See sensitivity analysis.

deuterium: An isotope of the element hydrogen with one neutron and one proton in its nucleus.

diffusion: The migration of particles in a gas, liquid, or solid from a region of high to low concentration (more accurately, from a region of high to low chemical potential) caused by random thermal (Brownian) motion of the particles.

diffusion coefficient: The ratio of the flux of a species to the driving force for diffusion, the gradient of concentration (more accurately, the gradient of chemical potential). The SI unit of measurement of diffusion coefficient is square metres per second (m^2/s).

discharge area: A portion of the earth's surface where the direction of flow of saturated groundwater is upward toward the water table. Also called discharge zone.

discrete variable: A random variable that can have only values belonging to a finite set or countably infinite set of possibilities.

dispersion: The combined effect of transport, diffusion and mixing that tends to distribute materials released from wastes or effluents through an increasing volume of water, air or soil, with the ultimate effect of diluting the materials.

disposal: A permanent method of long-term management of radioactive wastes in which there is no intention of retrieval and which, ideally, uses techniques and designs that do not rely for their success on long-term institutional control beyond a reasonable period of time.

disposal container: A durable receptacle for enclosing, isolating and handling nuclear fuel waste for disposal. In a disposal vault, the containers would serve as one barrier between the waste form and the human population. Sometimes called waste container or just container.

disposal facility: A disposal vault and the supporting buildings and equipment to receive the waste and package it in durable containers; shafts and equipment to transfer the containers from the surface to the vault; equipment to handle the containers in the vault; and the materials and equipment to excavate the vault, emplace the disposal containers and to fill and seal the vault, tunnels and shafts.

disposal system: 1. All structures, materials, processes, procedures or other aspects which, when taken together, constitute the means by which the safe disposal of waste is achieved. 2. In preclosure assessment, this includes a disposal facility and associated transportation facilities. 3. In postclosure assessment, it is a sealed disposal vault and its surrounding local geosphere and biosphere. See waste disposal system.

disposal vault: An underground structure excavated in rock for disposal of nuclear fuel waste. In the preclosure phase, the disposal vault would include the underground excavations in plutonic rock, the access shafts, access tunnels, underground service areas and installations, and disposal rooms. In the postclosure phase, it would include the disposal rooms and associated access tunnels, the nuclear fuel waste and the engineered barrier systems used to contain the waste and seal all openings. Also referred to as nuclear fuel waste disposal vault, nuclear waste disposal vault, used-fuel disposal vault, waste disposal vault and vault.

disruption scenario: As used in the postclosure assessment some feasible combination of factors (features, events and processes) that describe an unlikely situation in which some or all the engineered and natural barriers are significantly disrupted. It may include factors such as earthquakes and meteorite strikes. In our assessment of the reference disposal system, however, we conclude that only one such factor would be significant, and it is evaluated in the inadvertent human intrusion scenarios. Compare with the SYVAC scenarios.

distributed variable: A characteristic property of a system whose probability of being observed is described by a probability density function (for a continuous variable) or probability function (for a discrete variable).

distribution attribute: A characteristic of a probability density function (e.g., range, mean, standard deviation). One or more attributes may be required to completely define a probability density function; for example an unconstrained "normal" probability density function is often defined using its mean and standard deviation.

distribution coefficient (K_d): The concentration of a radionuclide sorbed on soil divided by its concentration in the associated groundwater. If used as a time-independent parameter, it is assumed that a sorption reaction is reversible and that equilibrium conditions prevail. The K_d approach is used to generate simplified models of radionuclide retardation resulting from a variety of processes that may include sorption, ion exchange, precipitation, diffusion into dead-ends, ultrafiltration, chemical substitution, complexation, speciation and colloid formation.

dose: A general term denoting the energy absorbed by a specified mass of a substance. Dose is often qualified to refer to specific quantities and to an individual versus a group of people or other biota. Examples of qualifications are: absorbed dose, dose equivalent, effective dose equivalent, committed effective dose equivalent, and collective dose. The SI unit of measurement of dose is the gray (Gy), although the sievert (Sv) is used when referring to dose equivalents to humans. In the EIS and the primary reference documents, dose is frequently encountered in expressions such as annual dose and dose per year. In these cases, it is an abbreviation of annual effective dose equivalent.

dose conversion factor: A multiplicative quantity used to convert intake of radioactivity to a committed effective dose equivalent (internal dose), or external exposure to radioactivity to an effective dose equivalent (external dose). The SI unit for the dose conversion factor is the sievert per becquerel (Sv/Bq) for internal doses, and Sv per unit of radionuclide concentration Sv/(Bq/L), Sv/(Bq/m^2) or Sv/(Bq/m^3) in the exposing media for external doses.

dose equivalent: The strict definition of radiological dose is the energy absorbed per unit mass of tissue exposed to ionizing radiation, measured in gray (Gy). The dose equivalent, measured in sievert (Sv), is the product of the dose and a radiation weighting factor. This weighting factor is a function of how a certain type of radiation deposits its energy within the body. Radiations with high weighting factors deposit a lot of energy in a short distance, whereas those with lower factors deposit less energy over the same distance. For example, alpha radiation has a weighting factor of 20, whereas beta and gamma radiations have a value of unity. See also radiological dose, effective dose equivalent and committed effective dose equivalent.

effective dose equivalent: The summation of the products of the dose equivalent that a particular tissue or organ has received and the corresponding organ weighting factor. This summation usually considers the entire body. The organ weighting factors are determined by the relative radiosensitivity of each organ. The effective dose equivalent is used to estimate the detrimental effect of a particular dose to the body, accounting for the fact that some organs are more sensitive to the effects of radiation exposure than others. In the postclosure report the unit of effective dose equivalent is sievert per year (Sv/a). See also radiological dose, dose equivalent and committed effective dose equivalent.

EIS: See Environmental Impact Statement.

element: Atoms that contain the same number of protons and that cannot be decomposed into any simpler units by any chemical transformation. Radioactive atoms spontaneously change into other elements by radioactive processes.

estimated annual dose: See ADE.

evaluation: The activity of assessing the reliability of a model through observations of real systems. Deciding that a model is suitable for a given application is a matter of expert judgment based on a knowledge of the requirements of the application, the characteristics of the model, and the nature of the observations made and the conclusions drawn from evaluations. Compare with validation and verification.

environmental and safety assessment: Evaluation of the behaviour and potential impacts of a disposal system, and comparison of the results with appropriate standards, regulations and guidelines. It includes evaluation of health impacts on humans and other biota. In the CNFWMP, the system under consideration is the entire disposal system, and one acceptability criterion is a limit on radiological risk to an individual of the critical group. Also referred to as the preclosure assessment and the postclosure assessment. The preclosure assessment considers impacts over the period of time covering the construction, operation and decommissioning of a disposal facility, up to and including the final shaft sealing and surface facility decommissioning. The postclosure assessment considers impacts starting after decommissioning, and extending far into the future.

Environmental Impact Statement (EIS): The documentation that records the results of the Canadian Nuclear Fuel Waste Management Program for assessing a waste disposal concept and the environmental impacts of its implementation. The documents conform with the Environmental Impact Statement documentation requirements specified in the federal Environmental Assessment and Review Process Guidelines Order.

equilibrium distribution coefficient (K_d): See distribution coefficient.

equilibrium surface distribution coefficient (K_a): The mass per unit surface area of a substance sorbed on a solid (mol/m^2), divided by its concentration in the associated solution (mol/m^3) after equilibrium is achieved. The SI unit of measurement is metre (m).

executive code: The main computer routines that control the calculations being performed, some of which may be carried out by dependent subroutines or functions invoked by the executive code. Also known as executive routines and executive program. In the series of codes involving SYVAC, the executive is the set of routines that oversees and controls the computation of system model code. For the computer code SYVAC3-CC3, the executive routines are frequently referred as SYVAC3.

expectation (symbol: E(X)): In statistics, the mean value of a distributed variable. Specifically, for a random continuous variable X with probability density function f(x), the expectation of X (i.e., the mean value of X), E(X), is

$$E(X) = \int_{-\infty}^{\infty} x\, f(x)\, dx \quad .$$

For a set of n randomly sampled values of x, an estimate of E(x) is the arithmetic average, or $\Sigma\, x_i/n$.

external dose: Quantity of radiation received from sources outside the body. The SI unit of measurement of dose is the sievert (Sv).

factor: In the postclosure assessment, this term has a specific meaning when used in association with scenario analysis. A factor is any feature, event, or process that could influence the performance of any component of the disposal system.

fission: The splitting of an atomic nucleus into two or more parts; may be spontaneous or induced by neutrons hitting the nucleus. Also called nuclear fission.

fission product: An atom produced either by nuclear fission or by the radioactive decay of an unstable atom produced by fission.

flux: The volume or mass of fluid or particles transferred across a given area perpendicular to the direction of flow per unit area in a given time. An example of the SI unit of measurement of flux is moles per square metre per second ($mol/m^2/s$).

fractional factorial analysis: A study of how the output of a model varies when all input parameters are restricted to a finite set of levels, rather than being allowed to take values from the full permissible range. For example, a two-level design restricts each parameter to two levels, usually a low value and a high value as determined by each probability density function. A full factorial analysis conducts simulations with all possible combinations of parameter values and analyses the results. A fractional factorial analysis uses a subset of these simulations, since the full factorial analysis usually requires an impossibly large number of simulations. The subset is usually chosen to optimize estimation of some statistics, such as the magnitude of the linear influence ("main effect") of each parameter.

free-water diffusion coefficient: The diffusion coefficient of a substance in pore water with no hindrance by a solid matrix. See diffusion coefficient.

gabbro: A coarse-grained, dark, igneous plutonic rock.

gamma radiation: The photons (gamma rays), which carry energy but no charge, emitted by an unstable atom. Gamma radiation is the most highly penetrating radiation. It can pass through the human body, but is stopped by a few centimetres of lead or a few metres of water or concrete. See also gamma ray.

gamma ray (γ): High-energy, highly-penetrating photons of short wave length commonly emitted by the nucleus of a radioactive atom during radioactive decay as a result of a transition from one of its excited energy levels to a lower level. Gamma radiation is the most highly penetrating radiation. It can pass through the human body, but is stopped by a few centimetres of lead, or a few metres of water or concrete.

genetic effect: A change induced by radiation in specific genes which manifests itself in the descendants of the exposed person.

GEONET: An AECL Whiteshell computer code that implements a GEOsphere model as a NETwork of segments through which contaminants move. It was written to serve as the geosphere model in SYVAC3-CC3, and is used in the postclosure assessment of the reference disposal system.

geosphere model: A model that describes transport of contaminants through fractured and porous rock that is saturated with groundwater. In SYVAC3-CC3, a waste disposal system is modelled using a system model that contains models for the vault, geosphere and biosphere. These models were introduced to simplify the development of mathematical models of complex processes. See also GEONET.

gradient: A vector whose direction is that of the greatest rate of change of a scalar property, such as temperature or contaminant concentration or hydraulic head, and whose magnitude is equal to the maximum value of the rate of change.

granite: A coarse-grained igneous rock consisting mostly of quartz (20 to 40%), alkali feldspar and mica. A number of accessory minerals may be present.

gray (Gy): The SI unit of absorbed dose for ionizing radiation. One gray is equal to 1 Joule of radiation energy absorbed in 1 kilogram of the material of interest. See also radiological dose.

groundwater: Water in the saturated zone beneath the earth's surface in soils and geologic formations.

groundwater velocity scaling factor: Factor for scaling groundwater velocities to describe uncertainty in the groundwater flow field. Velocities in all parts of the geosphere are scaled by the same factor to simulate the variation of hydraulic controlling parameters, such as permeability, without upsetting the overall water mass balance. Larger values of the scaling factor imply generally more water flowing in the geosphere. Contaminants are transported to the discharge locations more rapidly but with greater dilution. The well captures groundwater from a smaller distance, thus capturing less contaminants, to satisfy its required demand. Smaller values of the scaling factor have the inverse effect.

groundshine: Beta and gamma radiation emitted from radionuclides on the surface of the earth.

half-life, biological: The time required for the amount of a radioactive material present in a living organism to be reduced, by a combination of biological processes and radioactive decay, to one-half of its initial value. Biological processes dominate for long-lived radionuclides; radioactive decay dominates for short-lived radionuclides. The SI unit of measurement is second (s). Day (d) or year (a) are SI supplementary units and are also frequently used.

half-life, effective: See half-life, biological.

half-life, radioactive: Physical half-life is the length of time required for half of the original atoms in a material composed of a single species of radionuclide to decay to new atoms. Half-lives of different elements range from fractions of a second to billions of years. After a period equal to ten half-lives, the activity will have decreased to $(0.5)^{10}$ (about 0.1%) of its original value. The SI unit of measurement is second (s). Day (d) or year (a) are SI supplementary units and are also frequently used.

health effect: Fatal cancer or transmission of a fatal or debilitating genetic effect to offspring.

hold-up times: Characteristic periods of time describing the length of time that radionuclides would remain in plant and animal products and water. Hold-up times are used to estimate biological half-lives of radionuclides in materials used by the critical group. The SI unit of measurement is second (s). Day (d) or year (a) are SI supplementary units and are also frequently used.

hydraulic conductivity: The ratio of specific discharge to the force driving the flow of a viscous fluid flowing through a permeable medium. See Darcy's law. The hydraulic conductivity is a function of both the properties of the fluid and the properties of the permeable medium:

$$K = \frac{k\rho g}{\eta}$$

where K is the hydraulic conductivity, (m/s),
k is the permeability of the medium, (m^2),
ρ is the density of the fluid (kg/m^3),
g is the acceleration due to gravity (m/s^2), and
η is the viscosity of the fluid ($kg/(m \cdot s)$).

hydraulic gradient: In hydrogeology, the gradient of the hydraulic head. It is a dimensionless quantity, although frequently effectively dimensionless units such as metre per metre (m/m) are cited.

hydraulic head: In hydrogeology, a measure of potential at a point in a fluid. It is the sum of the pressure energy and the elevation potential energy per unit weight of the fluid. Hydraulic head is expressed as the height that the surface of a column of the fluid would stand above the point of potential measurement under atmospheric pressure measured from a reference datum point and has SI units of metres (m). A difference in hydraulic head between two points in the fluid is a driving force for fluid motion. The hydraulic head, the elevation, and the pressure are related by:

$$h = z + [p/(\rho . g)]$$

where h is the hydraulic head at the measurement point (m),
p is the pressure at the measurement point ($kg/(m \cdot s^2)$),
ρ is the fluid density (kg/m^3),
g is the gravitational acceleration constant (m/s^2), and
z is the elevation of the measurement point above a reference datum point (e.g. sea level) (m).

hydrodynamic dispersion: The spreading out of a solute caused by the movement of a fluid through a network of paths in a solid medium (e.g., fractures in granite). The hydrodynamic dispersion length is a parameter describing the magnitude of the spreading out of a solute carried by a fluid; it is scale-dependent and has SI units of metres (m). It is also known as dispersivity and hydrodynamic dispersion coefficient.

hydrostatic pressure: The pressure at some point in a motionless or uniformly flowing body of fluid exerted by the weight of the overlying fluid. It usually refers to a body of water such as as a lake or a saturated medium such as a pluton. Its SI unit of measure is kilogram per metre per square second ($Kg/(m \cdot s^2)$).

ICRP: See International Commission on Radiological Protection.

igneous: Formed by solidification of magma or lava.

impact: As used in the postclosure assessment, an effect on humans, nonhuman biota or the environment. The postclosure assessment evaluates only negative impacts, such as potential toxicity effects due to material that may be radioactive or chemically toxic.

impact assessment: Estimation of the future effects of a disposal system on humans and nonhuman biota, and evaluation of the results on the basis of standards and criteria. In this document, the preferred terms are postclosure assessment and preclosure assessment. See also environmental and safety assessment and performance assessment.

inadvertent human intrusion scenarios: As used in the postclosure assessment, radiation exposures initiated by human actions at the disposal site, following closure of the facility. These actions are unintentional, or inadvertent, in the sense that they are carried out without knowledge of the presence of a disposal vault and its potential hazards. The assessment of the reference disposal system evaluates two such actions in the inadvertent human intrusion scenarios: exposure of humans following a drilling operation to undispersed waste and to dispersed waste. (Three other types of inadvertent human intrusion are included with the SYVAC scenarios).

input parameter: A variable in a model (usually a computer model) which must be defined (input) before the model is used to generate a solution. In SYVAC simulations of a waste disposal system, one value of each input parameter is selected from the range of its possible values for each simulation.

iterated fractional factorial analysis: A method of sensitivity analysis in which fractional factorial designs are used to estimate the impact of changing each parameter. With large numbers of parameters, it is often easy to determine that variation of at least one parameter is having a significant effect, but difficult to identify which parameter is causing the effect. This problem is resolved in iterated fractional factorial analysis by performing many similar analyses (i.e. by iterating) until the truly significant parameters can be picked out with high confidence. If only a handful of parameters have significant effects, they can be identified from a set of simulation results containing fewer simulations than parameters. See fractional factorial analysis.

internal dose: Quantity of radiation received from sources inside the body. The SI unit of measurement of dose is the sievert (Sv).

International Commission of Radiological Protection (ICRP): An independent nongovernment expert body founded in 1928. This Commission establishes radiation protection standards that are followed by most countries.

intrusive: A term used to describe rock-forming materials that, while fluid, have penetrated into or between other rocks, and solidified before reaching the surface.

ion: An electrically charged atom or molecule. See atom.

ion exchange: Reversible movement of ions between a liquid phase and a solid phase that is not accompanied by any radical change in the solid structure.

ionizing radiation: Electromagnetic energy (e.g. X-ray or gamma-ray photons) or rapidly-moving atomic or subatomic particles having sufficient energy to displace electrons from atoms or molecules, thereby producing ions. Ionizing radiation may produce skin or tissue damage.

isotope: An atom. Different isotopes of an element have the same atomic number (or number of protons) but a different mass number (protons plus neutrons). Some elements have many isotopes. All isotopes of an element have the same chemical properties, but different physical properties. Radioactive isotopes are called radioisotopes.

LD1: In the postclosure assessment of the reference disposal system, a fracture zone that has been included to allow evaluation of the effects of such structures. Although based on investigations at the Whiteshell Research Area, many properties of LD1 are assumed. For example, it is assumed that LD1 starts at the overburden and, extends downwards past the plane of the vault, is connected at depth to a vertical joint, and is hydraulically well-connected to local recharge and discharge areas. The minimum distance from LD1 to the waste emplacement part of the nearest room is about 50 m, and is referred to as the waste exclusion distance.

lithostatic pressure: Pressure on an underground rock formation resulting from the weight of the overlying rock, soil, and water.

magma: Natural molten rock material generated within the earth.

mass number: The number of protons and neutrons in an atom.

mass loading coefficient for iodine: A parameter that accounts for all possible aquatic gaseous release mechanisms, as well as for effects of atmospheric dispersion. The ^{129}I air concentration is given by the mass loading coefficient for iodine multiplied by the ^{129}I concentration in lake water.

mass transfer coefficient: The ratio of the flux of a material crossing a boundary to the concentration difference of the material across the boundary layer.

matrix: With reference to nuclear waste, a material used to immobilize radioactive waste in a monolithic structure. Examples of matrices are bitumen, cement, various polymers, lead-antimony, glass and ceramic. For used nuclear fuel, the fuel pellets (mostly uranium dioxide) from a reactor are referred to as the fuel matrix or the UO_2 matrix.

mean (symbol: μ): The expectation or average value of a variable. For a continuous variable X with probability density function f(x), the mean is $\int_{-\infty}^{\infty} x\, f(x)\, dx$. For a discrete variable X with probability function f(x), it is $\Sigma\, x_i\, f(x_i)$, where the sum is over all possible values x_i of X.

mean, sample: A statistic applying to a sample of values of a variable. It is equal to the arithmetic average of the values, or $\Sigma\, x_i/n$, where the sum is over all n sampled values x_i of the variable. For very large values of n, the sample mean will approach the true expectation or mean of the variable.

median: For a distributed variable, the value about which there is an equal probability of selecting larger and smaller values. It is equivalent to the 50^{th} percentile or 0.5 quantile.

median-value simulation: A single simulation performed for deterministic analysis: all model parameters are given their median values (that is, the middle value or 50^{th} percentile of its probability density function). The median-value simulation is used to provide insight into how and where contaminants move within the reference disposal system, and it complements the probabilistic analysis of randomly sampled simulations.

medium: In waste disposal, the type of rock in which a disposal facility is located, and through which released waste must move to reach the surface environment.

migration: The movement of materials, e.g. radionuclides, through a rock medium or some other solid substance.

mode: For a distributed variable, the most probable value. For example, for a continuous variable X with a probability density function f(x), it is a value of X where f(x) is a global maximum.

model: An analytical or mathematical representation or quantification of a real system and the ways that phenomena occur within the system. Individual or sub-system models can be combined to give system models. In SYVAC3-CC3, for example, the system model consists of the vault, geosphere and biosphere models.

modelling: The creation or application of a mathematical representation of a physical, biological, or geological system. The mathematical representation is often converted into computer code so that the system can be examined in more detail.

Monte Carlo analysis: In applied mathematics, a probabilistic simulation method employing statistical sampling techniques to obtain an approximation to the solution of a complex problem for which an analytical solution is not available. The method requires repeated random selection of values of a large number of parameters defining contributing events and processes, and application of the mathematical theory of random variables.

MOTIF: Model Of Transport In Fractured/porous media, an AECL Research, Whiteshell Laboratories' computer program for predicting mechanical behaviour, fluid flow, heat transport, and solute transport in fractured/porous rock formations.

natural analogue: Situations in nature that parallel features of man-made structures, e.g., radioactive minerals or mineral deposits whose history of movement in groundwater over very long times can be determined and used to forecast the possible behaviour of chemically similar radionuclides in a disposal vault over a similar time frame.

natural background dose equivalent: The total radiation dose equivalent received from environmental sources, which include cosmic rays (from outside the solar system and from the sun), and radionuclides in the earth's crust, in the air, and in the human body. The SI unit of measurement of dose equivalent is the sievert (Sv).

natural background radiation: The various types of radiation not made by man, including: 1. External sources of extraterrestrial (cosmic rays) and terrestrial origin (the radioactive isotopes present in the crust of the earth, the water and the air), and 2. Internal sources, i.e., the radioactive isotopes of potassium and carbon, which are normal constituents of the human body, and other isotopes, such as ^{226}Ra and ^{232}Th and their decay products, which are ingested from the environment and retained in the human body.

neutron: An atomic particle with electric charge 0 and mass equal to 1.67×10^{-27} kg.

neutron activation: A nuclear process in which the nucleus of an atom captures a neutron. The resultant atom will have an increased atomic mass, and it may be either stable or radioactive. For example, hydrogen-1 can capture a neutron to form stable hydrogen-2 (also known as deuterium); hydrogen-2 can capture a neutron to form radioactive hydrogen-3 (also known as tritium).

node: Unique location in the transport network of the GEONET geosphere model defined by its spatial coordinates. Nodes are used to define the inlet and outlet locations of segments of the network.

nuclear fission: See fission.

nuclear fuel waste: A solid, highly radioactive material that is either the used nuclear fuel that has been removed from a Candu nuclear power reactor or a waste form incorporating the highly radioactive waste that would be removed from the fuel if the fuel were to be reprocessed.

nucleus (plural: nuclei): The positively charged core of an atom, with which is associated practically the entire mass of the atom, but only a minute part of its volume.

nuclide: A species of atom characterized by its mass number, atomic number and energy state.

open-borehole scenarios: As used in the postclosure assessment of the reference disposal system, scenarios involving the postulated presence of one or more open and unsealed boreholes drilled from the surface towards the disposal vault and passing close to a vault room containing nuclear fuel waste. Although the engineering design of the disposal system includes the permanent sealing of all boreholes, the possibility and consequence of an open borehole is examined in these scenarios.

packed particulate container: A used-fuel disposal container featuring a thin, corrosion-resistant metal shell supported by particles (such as glass or ceramic beads) filling the residual spaces between fuel bundles.

parameter: A characteristic of a system. In SYVAC simulations, a variable which has a constant value for a given set of assumed conditions (e.g., for one simulation) but which may be different for other conditions. In most applications of SYVAC to date, parameters remain constant throughout a specific simulation, but can be changed between simulations.

pathway: The route taken by contaminants from the containers in the vault, through the geosphere to a discharge area, and through the biosphere to where they impact the critical group or other biota. May also refer to specific routes within the biosphere, such as the plant-to-milk pathway in the food chain of the critical group.

PDF: See probability density function.

percentile: The k'th percentile of a cumulative distribution function for a variable X is the smallest value of x such that the probability of X not exceeding x is k/100. That is, the k'th percentile is the smallest solution to the equation $F(x)=0.01k$, where $F(x)$ is the cumulative distribution function of X. The fraction k is called the quantile.

performance (of a waste disposal system): The ability of a waste disposal system to isolate waste, and retard and disperse eventual releases of waste. One can refer to the performance of different parts of the system. For example, the performance of a container may refer to the period of time that the container remains intact and prevents the release of nuclear waste.

performance analysis: Development, testing and application of quantitative models for calculating or predicting the behaviour of a disposal system or subsystem in terms of a particular measure or measures.

performance assessment: Critical appraisal or evaluation in terms of one or more performance standards. For a disposal system this would mean evaluation of the behaviour of the system or subsystem, and comparison of the results with appropriate standards or criteria. It would be equivalent to a safety assessment if the system under consideration was the entire disposal system, and the performance measure was radiological impact or some other global measure of impact. For example, in the CNFWMP the system under consideration is the entire disposal system and one measure of performance is radiological risk to members of the critical group.

performance measures: Quantitative criteria for judging the behaviour of disposal systems or subsystems. Two examples are the risk to individuals caused by a disposal vault, and the time over which a disposal container remains intact.

performance targets: Specified levels of behaviour to be achieved, usually numerical values of selected measures of behaviour. For example, a disposal container might be required to have a lifetime of 500 a.

permeability: A geometric property of a porous rock, sediment or soil that affects its ability to allow passage of a fluid. The degree of permeability depends on the size and shape of the pores and on the size, shape and extent of the interconnections between the pores. Its SI unit of measurement is square metre (m^2). See hydraulic conductivity.

photon: A quantum of electromagnetic energy.

plant/soil concentration ratio: The ratio of nuclide concentration in plant material to that in soil. It quantifies the transfer of nuclides from soil to plants under steady-state conditions or at the time of harvest.

pluton: An intrusive body of igneous rock formed beneath the surface of the earth by consolidation of magma. Similar to batholith except that it is smaller in size.

plutonic rock: Intrusive igneous rock formed at considerable depth beneath the surface of the earth by cooling of magma. Also called intrusive igneous rock and crystalline rock.

porosity: The ratio of the aggregate volume of voids in a porous medium to its total volume. It is a dimensionless quantity, often expressed as a percentage, although it may sometimes be given with effectively dimensionless units such as cubic metre per cubic metre (m^3/m^3). In hydrogeology it usually refers to connected porosity.

postclosure: See postclosure phase.

postclosure assessment: Safety analysis of the waste disposal system, starting after the disposal vault has been closed. The objectives are to determine the long-term impacts of the disposal facility, and to provide estimates of risk that can be compared with regulatory criteria, standards and guidelines. See also performance assessment.

postclosure phase: In the CNFWMP, the project phase following the closure stage for a disposal facility, after the underground facilities have been decommissioned and sealed, the monitoring systems whose continued operation could affect long-term disposal vault safety have been removed, and the surface facilities have been decontaminated and decommissioned.

precipitation: In chemistry, formation of a separable solid phase within a liquid, removing dissolved material from solution. In meteorology, the fall of water in solid or liquid state onto the earth's surface.

preclosure: See preclosure phase.

preclosure phase: In the CNFWMP, the project phase that includes the siting, construction, operation, decommissioning and closure of a disposal facility including the disposal vault, surface facilities and surrounding site. It also includes the final shaft and monitoring borehole sealing. The transportation of used nuclear fuel from nuclear generating stations to the disposal facility is also part of the preclosure phase.

preclosure assessment: Safety analysis of the waste disposal system that deals with potential impacts during construction, operation, decommissioning and closure of a disposal facility. It includes an assessment of the transportation of used nuclear reactor fuel from nuclear generating stations to the disposal facility.

probabilistic analysis: A statistical method for studying the behaviour of a system defined in terms of parameters whose values are given as probability distributions, events whose occurrences are random and/or features which may or may not be present. The analysis gives a corresponding probability distribution of results. When the method of analysis used involves random sampling, it is often called Monte Carlo analysis, stochastic analysis, systems variability analysis or probabilistic safety assessment. Compare to deterministic analysis.

probabilistic sensitivity analysis: See sensitivity analysis.

probability: A measure of the degree of belief or frequency of observing the value of a variable in a particular interval (for a continuous variable), or equal to one of a set of discrete values (for a discrete variable). An absolute probability is defined with respect to an exhaustive list of the possible values of the variable; relative probabilities are defined with respect to one another. Frequentist (or objective) probabilities refer to the expected frequencies of observing different values by continuing a series of identical experiments or samplings; subjective probabilities are defined as the subject's degrees of belief that each of the possible different values will be the value that is observed in a single future observation.

probability density function (PDF): In statistics, a function f(x) of a continuous random variable X, whose integral over a particular interval gives the probability that the observed value of the variable will fall within that interval. Correspondingly, the probability function for a discrete variable X is a function f(x) whose sum for a set of selected values $\{x_i\}$ gives the probability that X has one of those values.

probability distribution: For a continuous random variable the integral of the probability density function (see cumulative distribution function). For a discrete variable, the set of probabilities of observing each of the possible values of the variable.

progeny: See daughter product.

proton: An atomic particle containing one positive unit of charge and with mass equal to 1.67×10^{-27} kg.

QA: See quality assurance.

quality assurance: Procedures used to provide evidence to demonstrate that the stated degree of quality in a product has, in fact, been achieved. It includes all those planned or systematic actions necessary to provide adequate confidence that a product or service will satisfy given needs. In the CNFWMP, the postclosure assessment has followed quality assurance procedures in the development of models, data and computer software, notably for SYVAC3-CC3.

quantile: The value of a variable corresponding to a particular point on its cumulative distribution function, that is, corresponding to a particular fraction of its total probability. See also percentile.

radiation: The very fast nuclear particles and/or photons emitted by nuclei, often taken to be synonymous with ionizing radiation. The four major forms of radiation are alpha and beta particles, neutrons and gamma rays.

radioactive: Emitting radiation. See radiation.

radioactive decay: The changing and progressive decrease in the number of unstable atoms in a substance, due to their spontaneous nuclear disintegration or transformation into different atoms, during which particles and/or electromagnetic radiation are emitted. Also called decay.

radioactive decay chain: A series of unstable (radioactive) nuclides. Each radionuclide in a decay chain produces daughters or progeny by spontaneous disintegration or radioactive decay. There are three long radioactive decay chains found in nature. The starting nuclides are generally taken to be the actinides ^{238}U, ^{235}U and ^{232}Th. In a nuclear reactor, a fourth long radioactive decay chain occurs due to neutron activation of the actinides; its starting nuclide may be taken to be ^{237}Np. The final member of these series, usually an isotope of lead, is stable. Other (generally shorter) radioactive decay chains may form during the fissioning process.

radioactive source term: 1. In an analysis of the movement and transfer of radionuclides in the environment, the activities and amounts of the different radionuclides per unit time leaving a nuclear installation or facility and entering the environment or an environmental compartment. 2. Information about the actual or potential release of radioactive material from a given source, which may include a specification of the composition, the amount, the rate and the mode of release.

radioactivity: The spontaneous emission of radiation, either directly from unstable atomic nuclei, or as a result of a nuclear reaction.

radiological dose: The strict definition of radiological dose is the energy absorbed per unit mass of tissue exposed to ionizing radiation, measured in gray (Gy). However, the terms radiological dose, or simply dose, are commonly used in different ways. They are also used as abbreviations for dose equivalent, effective dose equivalent, committed effective dose equivalent and collective dose in units of Gy, Gy/a, Sv, Sv/a and person-Sv.

radiological impact: As used in the postclosure assessment, this term generally refers to the estimated annual dose and consequent health risks from exposure to radiation.

radiological risk: The probability that a serious health effect will be suffered by an individual of the critical group or by his or her descendents. The risk is to be calculated as the sum over all significant scenarios of the product of the probability that the scenario will occur, the annual dose that would be incurred by an individual in the critical group if the scenario were to occur, and the probability of a serious health effect per unit dose (specified as 0.02 per sievert in AECB Regulatory Document R-104). See also risk.

radiolysis: The chemical decomposition of molecules by the action of ionizing radiation.

radionuclide: An unstable nuclide that undergoes radioactive decay.

radionuclide flow: The mass of a radionuclide moving past some boundary; it is frequently calculated by integrating the radionuclide flux over the area of the boundary. In SYVAC3-CC3, for example, the atmospheric models use the area-integrated flux of airborne radionuclides to a portion of the earth's surface (soil, vegetation, or water) as a result of deposition. The SI units of measurement flow is normally moles per second (mol/s); radionuclide flows are frequently given as becquerel per second (Bq/s).

radionuclide migration: The movement of radioactive species through various media due to fluid flow and/or diffusion.

random: Having no discernible pattern.

random variable: A numerically valued function defined on a sample space. Often random variables are defined on sample spaces associated with experiments in which the outcome of any one experiment is uncertain and is therefore said to depend on chance.

recharge zone: An area or portion of the earth's surface where saturated groundwater flow is generally downward.

reference container: The container evaluated in the postclosure assessment. It is an enclosed cylindrical vessel of titanium alloy which would hold 72 bundles of used nuclear fuel. Glass or ceramic beads would be compacted around the fuel bundles inside the container to support the container walls. See also packed particulate container.

reference disposal system (or reference system): The hypothetical disposal system that has been evaluated in the postclosure assessment. The reference system is a specific (but hypothetical) implementation of the concept for disposal of Canada's nuclear fuel waste. It includes a number of assumptions that are needed to facilitate the postclosure assessment. For example, the geological and hydrological characteristics of the reference disposal system are taken from information available on the Whiteshell Research Area, and the containers are assumed to be made of a titanium alloy. Models representing the reference system take into account all factors that were identified as important by scenario analysis.

reference man: A model of a hypothetical 'average' person for whom anatomical and physiological characteristics and data are specified in the report of the ICRP Task Group on Reference man (ICRP Publication No. 23 (1975) and IAEA Safety Guides, Safety Series No. 76). Its name notwithstanding, reference man includes both male and female characteristics relevant to calculation of radiological dose. The age of reference man is defined as 20 to 30 years. To permit the calculation of infant dose, the models and data for reference man were adapted for a one-year old (Johnson and Dunford, 1983). The model is used to estimate the radiation dose to the human body, whether from external or internal sources.

release: In waste management, the discharge of contaminants to the near surface environment where their effect may be detrimental.

response function: A Green's function, giving a mathematical solution to a differential equation with specified boundary conditions, where one of the boundary conditions is expressed as a Dirac delta function. It is used in SYVAC3-CC3 with the convolution method to find solutions for ordinary differential equations (which appear in compartment models used in the biosphere model) and for partial differential equations (which appear in mass transport equations in the vault and geosphere models).

retardation: see retardation factor.

retardation factor: Ratio of the speed of substances migrating in a fluid to the speed of the fluid itself; always less than or equal to unity.

retention: In dose modeling, the process whereby radioactive material is deposited in the human body, or in some organ of interest, and some of the material remains at any given time after deposition. The retention fraction is the fractional amount of radioactive material incorporated into tissues and organs.

risk: The term risk is commonly used in different ways and is understood in different ways by various segments of society. In technical terms, as used by AECL Research, risk is the probability that a serious health effect will be suffered by an individual. In the postclosure assessment, a measure of the expected harm that may result from the activities associated with nuclear fuel waste disposal. For radiological impacts, risk is defined by the AECB to be the "probability that a fatal cancer or serious genetic effect will occur to an individual or his or her descendants. Risk, when defined in this way, is the sum over all significant scenarios of the products of the probability of the scenario, the magnitude of the resultant dose and the probability of the serious health effect per unit dose". In mathematical terms:

$$\text{Risk} = \Sigma\, p_i \times d_i \times k$$

where p_i is the probability of occurrence of scenario i (dimensionless),
d_i is the estimated dose per year in scenario i (Sv/a), and
k is the risk factor, giving the probability of serious health effect per unit dose (probability of health effects/Sv). The AECB recommends a value of k equal to 2×10^{-2} serious health effects per sievert (AECB Regulatory Document R-104).

The summation extends over all significant scenarios i, and the unit of risk is the probability of a serious health effect per year (1/a).

risk analysis: A quantified examination of the hazards associated with a practice wherein the possible events and their probabilities of occurrence are considered together with their potential consequences, the distribution of these consequences within the population(s) affected, their distribution over time, and the uncertainties of these estimates.

risk factor: A quantity used to convert dose to risk. The AECB risk factor of 2×10^{-2} serious health effects per sievert (AECB Regulatory Document R-104) is used to quantify the risk that an individual will die from cancer or transmit a serious genetic effect to their offspring; the figure represents an average over age, sex and susceptibility.

safety assessment: Critical appraisal or evaluation in terms of one or more safety standards. In the CNFWMP, the system under consideration is the entire disposal system, and one acceptability criterion is a limit on radiological risk to individuals of the critical group. See also environmental and safety assessment and performance assessment.

safety criteria: Standards or criteria used to judge the acceptability of the protection afforded people and the environment. In the postclosure assessment, one safety criterion is a limit on radiological risk to an individual of the critical group.

sample: In probabilistic analysis, the process of assigning a value to an input parameter; this process may occur one or more times. For example, SYVAC selects values of a parameter from its probability density function using a random number generator, to generate a set of randomly chosen values. "Sample" may also be used as a noun, where it describes a set of values for one or more parameters selected from their probability distribution functions (for input parameters) or calculated based on an underlying model (for dependent parameters).

sampled parameter: In SYVAC, a parameter whose value is selected from a probability density function.

saturated: In hydrology, rock or soil whose void spaces are filled with water. In chemistry, a solution in which no more of a material can be dissolved.

SCEMR: Soil Chemical Exchange and Migration of radionuclides, an AECL Research computer program that models the movement of nuclides in soils. It was used to develop the soil submodel in the BIOTRAC code.

scenario: In the postclosure assessment, a set of factors (features, events and processes) that could affect the ability of the disposal facility to immobilize and isolate nuclear fuel waste. The SYVAC scenarios describe the expected behaviour of the disposal system and involve groundwater-mediated processes. Alternative scenarios define less probable, but potentially significant situations. Other possible scenarios that might be defined include a worst case scenario, which is intended to represent the most severe situation conceivable on the basis of pessimistic assumptions. Agreement on what constitutes a credible and meaningful worst case may be difficult.

scenario analysis: In the postclosure assessment, a systematic and comprehensive study to identify all sets of factors that must be considered in the assessment process. The two main functions are: 1. To identify and define all factors (features, events and processes) that could affect the performance of the disposal facility; and 2. To provide a systematic framework within which the importance of each factor may be evaluated. See also SYVAC scenarios.

sector: A portion of the disposal vault, treated as a unit in the transport calculations, having different properties from other sectors of the vault. Each vault sector releases contaminants at one node in the transport network of the geosphere model. Each geosphere node acting as a source for the transport network receives contaminants from only one vault sector.

segment: A portion of the transport network of the GEONET model with uniform chemical and physical properties. A segment is treated as a one-dimensional transport pathway between its inlet and outlet. The location of a segment is defined by the location of its inlet and outlet nodes.

sensitivity analysis: A quantitative examination of how the behaviour of a system varies with change, usually in the values of the governing parameters. Two common ways of varying input parameters are: 1. deterministic sensitivity analysis in which the parameters are varied only slightly about reference values (usually the median in this document). The intent is to determine the partial derivative of some output variable with regard to a single parameter. 2. probabilistic sensitivity analysis in which all parameters vary across their distributions or even change distributions. The goal of probabilistic sensitivity analysis is to determine the average impact of a parameter change in circumstances where other parameters are free to vary across their ranges also. See fractional factorial analysis.

sievert (Sv): The SI unit of dose equivalent. 1 Sv = 1 Joule per kilogram.

simulation: 1. In general terms, mimicking some aspect of the behaviour of one system with a different system. With reference to SYVAC, representation of the performance of a waste disposal system by the solutions to a set of mathematical models. 2. A time history of the models in SYVAC describing a release of substances from a waste disposal system and the resulting radiological or toxicological consequences to humans and the biosphere. In SYVAC3-CC3, a simulation is a single execution of the vault, geosphere and biosphere models for some set of unique values of the input parameters; this produces a single estimate of the consequences. In a deterministic simulation, the input parameter values are fixed beforehand. In a probabilistic simulation, the input parameter values are randomly sampled from their probability density functions.

simulation analysis: A general method for studying the behaviour of a real system or phenomena. It usually involves devising a mathematical model that represents the essential features of the system and solving the mathematical and logical relations of the model. The simulation can be either deterministic or probabilistic, depending on the model selected. The SYVAC3-CC3 computer code uses the Monte Carlo analysis method for its probabilistic (stochastic) simulations.

simulation cut-off time: In SYVAC3-CC3 calculations, the length of time, starting from closure of a disposal vault, for which release and transport of waste are simulated and consequences calculated. To satisfy Atomic Energy Control Board requirements, simulations using predictive mathematical models must be used for at least 10 000 a following closure.

SI unit: One of the standard quantities of measure (based on the metric system) in the international system (Système International) of units for scientific measurements.

somatic radiation effects: radiation-induced biological changes that would occur to the organism exposed, but would not be genetically propagated.

sorption: A broad term referring to reactions taking place within pores or on the surfaces of a solid. For contaminants being transported in groundwater through geological media, sorption could greatly reduce the rate of contaminant transport relative to the rate of groundwater transport. See also retardation and adsorption.

sorption capacity: A measure of the ability of a medium to sorb or chemically retain substances.

speciation: The chemical form (or mixture of forms) of a substance.

specific activity: 1. The number of disintegrations per second per unit mass of a pure radionuclide. 2. The number of disintegrations per second of a radioisotope per unit mass of that element present in the material. 3. The number of disintegrations per second per unit mass or volume of any sample of radioactive material.

Note: specific activity is commonly expressed in a wide variety of units, and care must be exercised in defining units.

specific discharge: The flux of fluid through a medium (m/s). It is equivalent to Darcy velocity. See also Darcy's law.

standard deviation (usual symbol: σ): The square root of the variance, a measure of the spread of a distribution around its mean.

statistic: An estimate or item of information about some distributed variable obtained from a sample of its observed values.

stochastic: Of a random or statistical nature. In mathematics, pertaining to random variables.

stochastic event: A random occurrence that can be predicted only to the extent of the probability of its occurring when an observation is made. The term is applied to data on phenomena that take place over a span of time or space and whose behaviours appear to be intrinsically unpredictable.

submodel: The mathematical representation of a part of a system. For example, several submodels, written in a computer language, may be used to construct a more complex computer model.

switch: As used in the postclosure assessment, a parameter of the system model used to select one from a group of conditions or system features for a simulation. Each condition in the group has an assigned probability; taken together, these probabilities define the corresponding probability density function (PDF) of the switch. In randomly selected simulations, a value of the switch parameter is sampled from its PDF which then selects the corresponding condition.

In SYVAC3-CC3, for example, the garden used by the critical group could consist of different types of soils. The options considered are sand, loam, clay or organic soils, with probabilities of occurrence of, respectively, 0.57, 0.05, 0.24 and 0.14 (based on the areal extent of each soil type on the Canadian Shield and current agricultural preferences). These probabilities are used to define a simple PDF for the "soil type" switch parameter. The PDF is a weighted piecewise uniform distribution with four discrete values 1, 2, 3 and 4. The weights assigned to these values are, 0.57, 0.05, 0.24 and 0.14 respectively, (that is, in 100 simulations, a value of 1 would be chosen 57 times on average, etc.). In a randomly sampled simulation, if the sampled value for the soil type switch parameter is 1, then the soil type is assumed to be sand.

systems analysis: An analytical procedure to determine how a set of interconnected components or processes, whose individual characteristics are known, will collectively behave in response to a given input or set of inputs.

SYVAC: SYstems Variability Analysis Code, a family of computer programs written at AECL Research, Whiteshell Laboratories, to perform probabilistic calculations on the long-term performance of disposal systems. Several generations and versions of SYVAC have been produced to assess, for example, disposal of high-level waste in an underground vault or under seabed sediment, and low-level tailings from uranium mining and milling operations. Different generations are substantially different from one another. Three generations of SYVAC now exist; they are referred to as SYVAC1, SYVAC2 and SYVAC3. Different versions of code are only slightly different from one another; each SYVAC generation has several versions.

SYVAC3-CC3: SYstems Variability Analysis Code, Generation 3, with models describing the Canadian Concept, Generation 3. This computer program belongs to the SYVAC family, and is the name given to the program that was used in the postclosure assessment of the reference disposal system. It consists of the SYVAC3 executive code and the third generation of the vault, geosphere and biosphere models.

SYVAC scenarios: As used in the postclosure assessment, a comprehensive combination of factors (features, events and processes) that describe the behaviour of the disposal system over a time-scale of thousands of years. This combination of factors describes the most probable pathways for the release of contaminants from their engineered containment and their transport through the geosphere and biosphere. The SYVAC scenarios are represented by the SYVAC3-CC3 system model. A variety of switches were incorporated into the system model to represent different contaminant transport pathways. As a result, the SYVAC scenarios comprise several hundred different exposure routes. The open-borehole and inadvertent human intrusion scenarios are considered as alternatives to the SYVAC scenarios, and are based on low-probability events.

terrestrial animal transfer coefficient: The quantity of nuclide transferred to the terrestrial food type milk (milk and dairy products), mammalian meats and poultry (poultry and eggs) from feed or forage, drinking water, or soil under steady-state conditions or at time of slaughter.

titanium (Ti): A malleable and ductile metallic element resembling iron. The reference container studied in the postclosure assessment is fabricated from commercially pure titanium (ASTM Grade 2).

tortuosity: Tortuosity is a measure of the effective increased pathlength for diffusion that results from the winding (or sinuous or tortuous) nature of the pore space in a porous medium. It has a variety of definitions in the literature but as used in the geosphere model in SYVAC3-CC3, we define it as the ratio of the effective distance that contaminant particles must travel, along a sinuous path around the solid particles of the porous medium, between two parallel planes to the shortest distance between those planes. Tortuosity is a dimensionless factor that, with this definition, always has a value greater than unity. In SYVAC3-CC3, tortuosity does not affect contaminant movement by flowing groundwater but it does affect contaminant movement by diffusion.

transfer parameter: In the BIOTRAC (or the biosphere model in SYVAC3-CC3), a constant used to calculate the amount of a substance moving from one biological compartment to another in the environment.

transport: Mechanism of movement of substances. See migration.

tritium: An isotope of the element hydrogen with two neutrons in its nucleus.

uncertainty: The quality or state of being indefinite, indeterminate, doubtful, not clearly defined or not clearly known. For the disposal concept assessment, uncertainty may pertain to scenarios, models, parameters and model predictions. Uncertainty can be accounted for through conservative assumptions and probabilistic assessment methodologies as in SYVAC. Uncertainty may include spatial and temporal variability.

uncertainty analysis: A quantitative evaluation of the possible variability and error in quantities involved in, or results obtained from, solving a problem. One approach to uncertainty analysis is known as probabilistic analysis. This involves defining the input data in probabilistic form and applying statistical techniques to the results.

validation: The process by which one provides evidence or increased confidence that a model is adequate for the purpose for which it is used. It is commonly regarded as a procedure that involves comparison of the predictions of a model with observations of a real system. A conceptual model is considered to be validated when the comparison with measurements on a real system shows that it provides a sufficiently good representation of the actual processes occurring in the real system, in keeping with the intended use of the model. In the case of the postclosure assessment, the results from SYVAC3-CC3 apply to times up to 10^4 a and longer. This implies that validation cannot be achieved in full, because the operation of an actual disposal system cannot be observed over the time frame required to permit comparison with results from SYVAC3-CC3. There is also no direct analog known in nature that would permit a complete comparison with an actual disposal system. Nonetheless, different components of the model may be validated to some extent, through comparisons with experimental observations (generally covering short times spans) and with natural analogues (often covering long time spans). Compare with evaluation and verification.

variability: The quality or state of being not constant and subject to change, often in terms of space and time. For the disposal concept assessment, variability may pertain to aspects of physical, chemical or biological processes, as reflected in model parameters and predictions. Variability can usually be measured and quantified statistically. In probabilistic assessment methodologies, such as SYVAC, variability is expressed together with uncertainty so that the two cannot easily be distinguished.

variable: 1. In mathematics, a symbol representing a quantity. 2. In SYVAC3-CC3, a quantity that may change with time in a given simulation.

variance: The expectation of the square of the difference between the values of a distributed variable, X, and its mean, μ. For a continuous variable X with probability density function f(x), the variance is the integral of the function $(x - \mu)^2 f(x)$, evaluated over all possible values x of X. For a discrete variable with probability density function f(x), it is the sum of the function $(x_i - \mu)^2 f(x_i)$, evaluated over all possible values x_i of X.

variance, sample: A statistic applying to a sample of values of a variable. It is equal to the sum: $\Sigma (x_i - s)^2 / (n-1)$, where s is the sample mean of the set of n sampled values. For very large values of n, the sample variance will approach the true variance of the variable.

vault model: A computer model describing processes in the vault such as corrosion of metallic disposal containers and the transport of contaminants through the buffer. In SYVAC3-CC3, the disposal system is modelled using a system model that contains models for the vault, geosphere and biosphere. These models simplify the development of mathematical models of complex and unrelated processes.

verification: As used in the postclosure assessment, the process by which one provides evidence or increased confidence that a computer code correctly executes the calculations it is asserted to perform. A verified computer code is one that has correctly translated a specified algorithm into computer code. Verification can be carried out, for example, by comparing the results of a computer code with results produced by other computer codes or by analytical solutions. Compare with validation and evaluation.

viscosity: The property of a fluid whereby it tends to resist relative motion within itself. A highly viscous liquid drags in a molasses-like manner. Also known as internal friction. The SI unit of measurement of viscosity is newton-second per square metre ($N \cdot s/m^2$).

waste disposal system: The engineered systems (e.g., containers, buffer and backfilled tunnels and rooms, sealed shafts and boreholes) and natural surroundings (e.g., rock and rubble-filled fractures) and local surface biosphere involved in forestalling, retarding and minimizing the effects of any release of waste substances from permanent isolation.

waste exclusion distance: As used in the postclosure assessment of the reference disposal system, a region of rock that isolates the waste emplacement part of a vault room from fracture zone LD1. This region is achieved by modifying the location of the vault and by using shorter lengths for the vault rooms nearest LD1. The closest distance in a horizontal direction from LD1 to any room is about 155 m; however, the closest distance is only about 50 m because the plane of the fracture zone is not vertical, but inclined at a shallow angle to the plane of the vault. In the reference disposal system, therefore, the waste exclusion distance is about 50 m.

waste form: One of the forms of nuclear fuel waste: either used CANDU fuel or the solidified high-level waste from reprocessing.

<u>waste immobilization</u>: Conversion of radioactive waste to a solid form that reduces the potential for migration or dispersion of radionuclides by natural processes or accident during storage, transportation and disposal.

<u>water table</u>: In geology, the upper surface of a zone saturated with groundwater; the surface of a body of unconfined groundwater at which the pressure is equal to that of the atmosphere.

<u>Whiteshell Research Area (WRA)</u>: A tract of land located in the Whiteshell region of southeastern Manitoba, and near the Whiteshell Laboratories of AECL Research. Much of the information used in the postclosure assessment derives from research studies at the WRA. In particular, the geosphere model is based on detailed hydrogeological studies of the WRA.

<u>WRA</u>: See Whiteshell Research Area.

<u>Zircaloy</u>: A trade name for a family of alloys containing zirconium as the main constituent. Zircaloy is used to make the fuel cladding and structural components of reactor fuel bundles.

APPENDIX H

LIST OF ACRONYMS

ADE	Annual Dose Estimate
AECB	Atomic Energy Control Board
AECL	Atomic Energy of Canada Limited
ANSI	American National Standards Institute
BIOMOVS	BIOsphere MOdel Validation Study
BIOTRAC	BIOsphere TRansport And Consequence model
CANDU	CANada Deuterium Uranium
CEC	Commission of the European Communities
CNFWMP	Canadian Nuclear Fuel Waste Management Program
COG	CANDU Owners Group
CSA	Canadian Standards Association
DCF	Dose Conversion Factor
EARP	Environmental Assessment and Review Process
EIS	Environmental Impact Statement
EMR	Energy Mines and Resources Canada
ERL	Environmental Resources Limited
GEONET	GEOsphere NETwork model
GSC	Geological Survey of Canada
IAEA	International Atomic Energy Agency
ICRP	International Commission on Radiological Protection
IEEE	Institute of Electrical and Electronic Engineers
IFFA	Iterated Fractional Factorial Analysis
INTRACOIN	INTernational RAdionuclide transport COde INtercomparison study
MOTIF	Model Of Transport In Fractured porous media
NAGRA	NAtionale Genossenschaft für die Lagerung Radioaktiver Abfälle (Switzerland)
NATO	North Atlantic Treaty Organization
NEA	Nuclear Energy Agency (OECD)

NCRP	National Council on Radiation Protection (United States)
NRCC	National Research Council of Canada
OECD	Organisation for Economic Co-operation and Development
OME	Ontario Ministry of the Environment
PAGIS	Performance Assessment of Geological Isolation Systems
PDF	Probability Density Function
PSAC	Probabilistic Systems Assessment Code user group
PSAG	Probabilistic Systems Assessment Users Group
QA	Quality Assurance
SENES	Senes Consultants Limited
SKB	Swedish Nuclear Fuel and Waste Management Company
SKBF/KBS	Swedish Nuclear Fuel Supply Company, Division KBS
SYVAC3	SYstems Variability Analysis Code - generation 3
SYVAC3-CC3	SYstems Variability Analysis Code, generation 3 with the Canadian Concept models, generation 3, for the disposal of Canada's nuclear fuel waste
TAC	Technical Advisory Committee to AECL on the Nuclear Fuel Waste Management Program
UNSCEAR	United Nations Scientific Committee on the Effects of Atomic Radiation
URL	Underground Research Laboratory
US DOD	United States Department of Defense
UTAP	Uranium Tailing Assessment Program
WRA	Whiteshell Research Area
WL	Whiteshell Laboratories