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Performance Assessment of the Direct Disposal in Unsaturated Tuff of Spent Nuclear Fuel and High-Level Waste Owned by U.S. Department of Energy

Volume 2: Methodology and Results

Rob P. Rechard, Editor

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Volume 2: Methodology and Results

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Abstract

This assessment studied the performance of high-level radioactive waste and spent nuclear fuel in a hypothetical repository in unsaturated tuff. The results of this 10-month study are intended to help guide the Office of Environment Management of the U.S. Department of Energy (DOE) on how to prepare its wastes for eventual permanent disposal. The waste forms comprised spent fuel and high-level waste currently stored at the Idaho National Engineering Laboratory (INEL) and the Hanford reservation. About 700 metric tons heavy metal (MTHM) of the waste under study is stored at INEL, including graphite spent nuclear fuel, highly enriched uranium spent fuel, low enriched uranium spent fuel, and calcined high-level waste. About 2100 MTHM of weapons production fuel, currently stored on the Hanford reservation, was also included. The behavior of the waste was analyzed by waste form and also as a group of waste forms in the hypothetical tuff repository. When the waste forms were studied together, the repository was assumed also to contain about 9200 MTHM high-level waste in borosilicate glass from three DOE sites. The addition of the borosilicate glass, which has already been proposed as a final waste form, brought the total to about 12,000 MTHM.

A source term model was developed to study the wide variety of waste forms, which included radionuclides residing in 10 different matrices and up to 8 nested layers of material that might react with water. Several important capabilities of this model, which is embedded into a two-phase composite-porosity fluid flow and transport model, are approximations of diffusion through rubble contacting a container, wet/dry oxic/anoxic corrosion, retardation on corrosion products, separate solubilities for inside/outside container, and corrosion rate dependence on temperature, presence of oxygen, water saturation, and time, if desired. In most cases, information readily available in literature was used to develop approximately 3700 data items needed by the models; when new data were required for the detailed phenomenological modeling used in this study, subjective estimates from analysts were necessary. The use of subjective estimates is in keeping with the need to provide immediate guidance to DOE on its waste forms, although improved defensibility of the input data would be desirable.

1 The possibility and consequences of critical conditions occurring in or near containers of highly enriched
2 uranium spent nuclear fuel were also studied. Although a full coupling of conditions that control a criticality
3 occurrence was beyond the scope of this performance assessment, a range of temperature and water saturation
4 was considered in preliminary reactor dynamics calculations, in which phenomena were manually coupled.
5 Other analysis approaches included summarizing data from historical criticality accidents to bound
6 probable conditions and performing scoping calculations in which the repository was assumed to act like a
7 reactor at steady state.
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10 The criteria used to measure performance included disposal system criteria, with special emphasis on the
11 individual protection requirements, in the U.S. Environmental Protection Agency's *Environmental Radiation*
12 *Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic*
13 *Radioactive Waste*, 40 CFR 191 (although this standard has been set aside by the *Energy Policy Act of 1992*),
14 and the waste package and engineered barrier requirements in the Nuclear Regulatory Commission's *Dis-*
15 *posal of High-Level Radioactive Wastes in Geologic Repositories*, 10 CFR 60.
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19 The general findings are as follows: For a repository in unsaturated tuff, disposal of currently existing DOE
20 spent fuel and high-level waste, with minimal treatment or conditioning in a disposal container of carbon
21 steel and Incoloy Alloy 825, behave similarly to commercial pressurized water reactor fuel and high-level
22 waste in borosilicate glass. Furthermore, the waste complied with the overall dose and containment require-
23 ments of 40 CFR 191 over 10,000 yr. Technetium-99 was the major contributor to doses in the groundwater
24 pathway in the first 10,000 yr, but neptunium-237 was the most important at 100,000 yr. The small inven-
25 tory of carbon-14 in the DOE spent fuel helped in complying with the current containment requirements.
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29 The temperature of the repository peaked at slightly above 90°C and stayed above 80°C for about 1000 yr
30 when the containers were placed horizontally inside long tunnels with a power density of 23.5 W/m².
31 Because of the high corrosion rate associated with the high temperatures, the disposal container did not meet
32 the requirements of 10 CFR 60 even though the overall disposal system complied with 40 CFR 191. The
33 differences in behavior among the waste types were partially caused by the local differences in temperature
34 as the result of substantial differences in heat output per waste type. The cooler high-level waste performed
35 better than the hotter spent fuels. No substantial difference was seen between the loose and immobilized
36 calcine high-level waste currently stored at INEL.
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39 Although the criticality calculations are preliminary, they support the belief that it would be difficult to cre-
40 ate conditions that would provide enough water from infiltration in a 10,000-yr regulatory period to (a) cor-
41 rode the containers, (b) remove neutron absorbers or uranium, and (c) moderate a nuclear chain reaction.
42 Furthermore, should a criticality occur in or near a container in an unpressurized system at some future time,
43 the nuclear dynamic calculations show that such a critical condition is extremely sensitive to minute changes
44 in groundwater saturation that, in turn, are sensitive to changes in temperature. Therefore, it would be very
45 difficult to keep a natural reactor operating at a power level similar to that which occurred with aqueous
46 accidents. The calculations indicated that a noticeable increase in temperature lowered the saturation
47 enough to stop the nuclear reaction. Finally, the bounding calculations, which assumed a steady-state criti-
48 cality reaction similar to the low power of historical aqueous accidents, produces no more than 10²⁵ fissions
49 operating over 10,000 yr. Thus, should all 289 containers with highly enriched uranium fuel go critical for
50 10,000 yr, only about 10²⁸ fissions occur, which is less than a 1% increase to the fission products (radionu-
51 clide inventory) already existing in a 12,060-MTHM repository, given an average burnup of the spent fuel.
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1. Introduction

R. P. Rechard

1.1 Purpose

The purpose of this report is to provide information to the U.S. Department of Energy (DOE) about three specific topics related to waste disposal in the United States. First, an analysis is presented on the effects of disposal of spent nuclear fuel and high-level waste, which is owned by the DOE, under the following conditions: minimal treatment of the spent fuel and waste, use of currently proposed containers with both corrosion-allowance and corrosion-resistant layers, and disposal in a geologic repository in volcanic tuff. The intent is to provide information to the DOE about whether minimal treatment of the waste under these conditions would benefit or hinder compliance. Second, the analysis evaluates the probability and consequences of a critical condition developing in a closed and sealed tuff repository after disposal of the waste. Third, because the analysis procedure is similar to the method that is expected to be used for final compliance, the report provides information about the status of existing models, including deficiencies in either current modeling capabilities or existing data. Of particular note is the information provided about the models and data for corrosion and criticality, because neither topic has been extensively studied previously.

The performance assessment reported here is a continuation of an effort that was funded by the Office of Environmental Management of the DOE. The purpose of the initial study was to assist the DOE in evaluating whether treating spent nuclear fuel and high-level waste before disposal in a deep, geologic repository would contribute to the efficacy of the disposal method and thereby aid in compliance of the repository. The initial study considered five waste treatment options, ranging from no conditioning to a high level of treatment. In this study (referred to herein as the 1993 PA), two generic sites—one in salt and the other in saturated granite—were considered as repositories for the waste. A very general summation of the results of the 1993 PA is that the performance of the waste was tied most closely to the repository type, and that when differences in the waste treatment options were discerned, they were evident primarily between the minimal and maximal treatment options (Rechard, Ed., 1993).

Based on the results of the 1993 PA, the performance assessment reported here, referred to as the 1994 PA, examines one treatment option for five types of spent nuclear fuel and three treatment options for calcined high-level waste. The types of waste are graphite spent nuclear fuel, highly enriched uranium spent fuel, robust highly enriched uranium spent fuel, low enriched uranium spent fuel, weapons production fuel, and calcined high-level waste. Specific fuels that are being modeled to represent the spent fuels are from Fort St. Vrain, graphite; Advanced Test Reactor (ATR), highly enriched; Shippingport, robust highly enriched; pressurized water reactor (PWR), low enriched; and N-Reactor, weapons production. These wastes and spent fuels are currently stored at the Idaho National Engineering Laboratory (INEL) or the Hanford reservation. Two sets of analyses are performed in parallel: a Simple PA, in which only one waste type at a time is assumed in the repository, and a Complex PA, in which all waste types are in the repository. For the Complex PA, high-level waste in borosilicate glass from three DOE sites is included for comparison. The sites are the Savannah River Plant, South Carolina; the Hanford Reservation, Washington; and West Valley, New York.

The hypothetical repository for the 1994 PA is in unsaturated tuff, similar to the potential repository at Yucca Mountain, Nevada, to examine the effects of disposal of DOE spent fuel in a Yucca Mountain-like repository. Yucca Mountain is currently under consideration for disposal of commercial spent fuel and a portion of the defense high-level waste in the U.S. Tuff was not considered as one of the two repositories in the 1993 PA because the demands of creating the initial performance assessment were such that it was deemed prudent to concentrate on repositories with abundant site characterization data and a good understanding of physical processes, and thus delay modeling of an unsaturated tuff repository until the 1994 PA. Furthermore, the salt and granite disposal systems were thought to adequately bound the behavior of a generic disposal system.

As part of examining the response of an unsaturated tuff repository containing DOE spent fuel and high-level waste, the 1994 PA also studied the possibility of a critical condition developing in one or several containers of highly enriched uranium spent fuel. A study of criticality was strongly recommended by reviewers of the 1993 PA, who felt that limiting the amount of ^{235}U per waste parcel might be overly conservative. (In the 1993 PA, the amount of ^{235}U

1. Introduction

was limited to 0.7 kg in parcels for the granite repository and 10 kg in the salt repository to ensure that a criticality did not occur within a container; however the limit meant that an increased number of waste parcels was required for highly enriched uranium spent fuel.) The technical aspects of determining how a criticality can occur and its effects are complicated in a geologic repository because—unlike a nuclear reactor—the range of possible thermal-hydraulic conditions cannot be defined over time. Initial attempts to bound the effects of a criticality include steady-state scoping calculations, in which the repository is assumed to act like a reactor; data from historical criticality accidents; and reactor-dynamics calculations, in which a range of thermal-hydraulic input is considered.

In the 1994 PA, the performance criteria include (1) Containment Requirements and Individual Protection Requirements from 40 CFR 191, with an emphasis on maximum annual effective dose equivalent, and (2) technical criteria for the container and waste form as defined in 10 CFR 60. (Only 40 CFR 191 was considered in the 1993 PA.) As discussed further in Section 1.2, 40 CFR 191 no longer applies to repositories characterized under the Waste Policy Act (NWPA, 1983) and so a new standard is required. Also, 10 CFR 60 must be modified to agree with the future standard.

The process for the 1994 PA is the same as that used in 1993 which, in turn, is based upon the methodology developed for the performance assessment of the Waste Isolation Pilot Plant (WIPP) Project (see, for example, WIPP PA Division, 1991a, Chapter 3). Because site characterization was beyond the scope of this 10-month task, the 1994 PA also takes advantage of site characterization data from Sandia's Total-System Performance Assessment of the Yucca Mountain Project performed in 1993 (referred to as TSPA-1993) (Wilson et al., 1994). The repository and container designs, however, represent more current conceptual designs (TRW, 1993b). The waste characterization data for the 1994 PA were collected and interpreted by Lockheed Idaho Technologies Company (LITCO), the operator at INEL, and are presented in Appendix A. The 1994 PA calculational design is similar to the 1993 PA in that both a Simple and Complex PA are run, a technique that has proved particularly useful in establishing sensitive parameters for the assessment. The Simple PA takes advantage of codes used in TSPA-1993, while the Complex PA uses modified codes from the 1993 PA.

The remainder of this chapter expands upon the information just presented, outlines important concepts in the performance assessment, and highlights decisions that affect how the disposal system was modeled. Chapters 2 through 14 provide additional details on the concepts and assumptions presented here; Chapter 15 contains the results of the assessment. Appendices offer other background information about the waste, waste parcel contents, criticality events, regulatory criteria, scoping calculations, and modeling systems. Readers should turn to related chapters and appendices for detailed information about areas of interest.

1.2 Legal Setting

Several laws and regulations affect the disposal of radioactive waste in geologic repositories (Table 1-1). Two laws of particular importance in regard to defining policy are the *Nuclear Waste Policy Act of 1982* (NWPA, 1983) and the *Energy Policy Act of 1992* (Energy Policy Act, 1992). These laws and their effects on current plans for waste disposal are discussed below.

Despite these policy acts, however, regulations that establish performance criteria are not fixed. As described below, the Environmental Protection Agency's standard, *40 CFR 191: Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes* (EPA, 1985a; 1993) is undergoing review and is not expected to be repromulgated until 1996. Revision of the Nuclear Regulatory Commission's 10 CFR 60 is not anticipated until 1997.

Because the final regulations are still in flux, the 1994 PA considered the following performance criteria. Like the 1993 PA, the 1994 PA used the performance criteria defined in 40 CFR 191 for the whole system, including containment requirements and individual protection requirements. However, in response to preliminary guidance from the Energy Policy Act, the 1994 PA emphasized the individual protection requirements, which use maximum annual effective dose equivalent. Also, the 1994 PA considered the performance criteria for the container and waste form as defined in 10 CFR 60; this regulation was not considered in the 1993 PA. Current regulations regarding hazardous

Table 1-1. Selected Statutes and Regulations Affecting the Disposal of Radioactive Waste in Geologic Repositories

Policy Act or Regulation	Influence on Repository and/or Waste Treatment
<ul style="list-style-type: none"> Nuclear Waste Policy Act of 1982 Nuclear Waste Policy Amendments Act of 1987 	Set national policy on nuclear waste disposal
<ul style="list-style-type: none"> Energy Policy Act of 1992 (EPA) 	Set aside 40 CFR 191 and asked the National Academy of Sciences to recommend to the Environmental Protection Agency (EPA) standards for the Yucca Mountain repository site and requires the Environmental Protection Agency and the Nuclear Regulatory Commission to make subsequent revisions in their regulations for this specific site. The law strongly suggests the use of maximum annual effective doses to individuals.
<ul style="list-style-type: none"> Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Wastes, 40 CFR 191 Disposal of High-Level Radioactive Wastes in Geologic Repositories, 10 CFR 60 	Established long-term performance criteria for geologic repositories
<ul style="list-style-type: none"> Resource, Conservation, and Recovery Act of 1976 (RCRA) and Hazardous and Solid Waste Amendments of 1984 (implemented in 40 CFR 124 through 40 CFR 181) 	Potentially important in the establishment of long-term performance criteria
<ul style="list-style-type: none"> National Environmental Policy Act of 1969 (NEPA) 	

waste are also described in this section. A more thorough discussion of the current legal setting can be found in Chapter 2.

1.2.1 Nuclear Waste Policy in the United States

The *Nuclear Waste Policy Act of 1982* (NWPA, 1983) and subsequent amendments of 1987 (NWPA, 1987) establish a national policy for interim storage, monitored retrievable storage, and eventual disposal of radioactive waste. Although performance criteria are not established, the act does specify the approach to nuclear waste disposal to be followed in the United States. The policy is based on the belief that the current generation has an obligation to bear the political and financial costs of developing a permanent disposal option. A specific requirement that directly affects disposal of the waste considered in the 1994 PA is that DOE defense and experimental waste, with the exception of defense transuranic waste, should be disposed of with commercial waste and thus must comply with all requirements of the Nuclear Regulatory Commission (NRC).

The *Energy Policy Act of 1992* (Energy Policy Act, 1992) set a new policy that has generated substantial changes in the regulatory setting. The act requires a site-specific standard for the proposed nuclear waste repository at Yucca Mountain, Nevada, and strongly suggests maximum annual effective dose equivalents as the criteria for protecting public health. Specifically, the Energy Policy Act (1) directs the National Academy of Sciences (NAS) to examine (a) the usefulness of annual effective dose equivalents as a standard, (b) whether institutional controls can reasonably prevent unreasonable risk of intrusion into the repository, and (c) whether scientifically supportable predictions beyond 10,000 are possible; (2) sets aside the EPA standard, 40 CFR 191; (3) requires promulgation of a new standard, including prescription of maximum annual effective dose equivalents, based on recommendations by the NAS; (4) states that the new EPA standard will be the only standard applicable to Yucca Mountain; and (5) requires revision of the NRC regulation, 10 CFR 60, to (a) agree with the new EPA standard and (b) assume that post-closure oversight

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at the repository will prevent unreasonable risk of breaching the repository, consistent with recommendations by the NAS.

The NAS study is expected in April 1995; promulgation of the new EPA standard is required within one year from the NAS study, and revision of 10 CFR 60 is required a year later.

1.2.2 40 CFR 191, EPA Standard

In 1985, in response to the Nuclear Waste Policy Act, the EPA promulgated the standard, *40 CFR 191: Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes* (EPA, 1985a; 1993), which had been under study since 1977. However, the regulation was remanded shortly thereafter and then repromulgated in 1993, as directed by the Waste Isolation Pilot Plant Land Withdrawal Act (WIPP LWA, 1992). Although 40 CFR 191 initially applied to all deep geologic disposal on land, this standard now defines criteria for radioactive waste disposal, based on a total system program, only for repositories *not* characterized under the Nuclear Waste Policy Act (NWPA, 1983).

In the 1994 PA, two criteria from 40 CFR 191 were used: (1) the Containment Requirements, which are probabilistic limits on summed releases for 10,000 yr for the entire disposal system, and (2) the Individual Protection Requirements, which place limits on the mean maximum annual effective dose equivalent received by individuals from instantaneous releases from the disposal system over 10,000 yr at 150 μ Sv/yr. As the result of using these criteria in the 1994 PA, a stochastic analysis was necessary to evaluate instantaneous and summed releases at the disposal system boundary for 10,000 yr. (See also Section 1.8, Regulatory Assessment.)

A more thorough discussion of 40 CFR 191 is provided in Chapter 2. Appendix C contains the preamble to 40 CFR 191, as promulgated in 1985, and the current text of 40 CFR 191, as repromulgated in 1993.

1.2.3 10 CFR 60, NRC Regulation

The EPA standard, 40 CFR 191, establishes standards for the disposal system as a whole to protect the accessible environment. However, the NRC is responsible for ensuring that a DOE disposal system for commercially generated spent fuel and high-level radioactive waste meets the requirements of EPA's 40 CFR 191. Prior to passage of the Nuclear Waste Policy Act of 1982, the NRC had promulgated the licensing portion of *10 CFR 60—Disposal of High Level Radioactive Wastes in Geologic Repositories* (46 FR 13971) (NRC, 1981). In June, 1983, several months after passage of the NWPA, the NRC promulgated the technical criteria for 10 CFR 60 in order to evaluate the suitability of a geologic repository (NRC, 1983a).

The NRC anticipated the promulgation of the EPA standard and "implemented" it by incorporating it into the agency's regulations. Yet in the technical criteria the NRC also established minimum requirements for the engineered and geologic barrier subsystems of the disposal system (treating the disposal system like a nuclear reactor) that required compliance calculations (BRWM, 1992, p. 7). The requirements are stringent: a period for substantially complete containment of radionuclides by the waste packages (may vary from a minimum of 300 yr to a maximum of 1000 yr); a maximum engineered barrier release rate (1×10^{-5} /yr of the 1000-yr inventory after the containment period for any radionuclide released at a rate greater than 0.1% of the calculated total release rate limit); and a minimum 1000-yr groundwater travel time from the repository to the accessible environment (prior to construction) for the geologic barrier. Thus, the requirements for compliance with 10 CFR 60 potentially require the implementing agency to have a much more thorough understanding of the engineered and geologic subsystem than for 40 CFR 191.

In addition to these performance criteria, 10 CFR 60 also flatly prohibits some waste forms. In §60.135, it states "particulate waste forms shall be consolidated (for example by incorporating into an encapsulating matrix) to limit the availability and generation of particulates." Thus, calcine must be treated even though the 1993 PA indicated that calcine was an adequate waste form without encapsulation. Because of this requirement, the "base case" form of cal-

1 cine in the 1994 PA is encapsulation in glass-ceramic rather than loose calcine grains as was modeled in the 1993 PA.
 2 (See also Section 1.8, Regulatory Assessment.)
 3

4 A more thorough discussion of 10 CFR 60 is provided in Chapter 2. Appendix C contains the preamble to the
 5 technical criteria as promulgated in 1982 and the current text of 10 CFR 60.
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10 1.2.4 Hazardous Waste Standards

11 According to current definitions, the waste types modeled in the 1994 PA are considered to be mixed waste. The
 12 calcine high-level waste from INEL is considered as mixed because hazardous chemicals from hot cells at the Chem
 13 Plant were included in the liquid high-level waste during reprocessing. Also, although spent fuel is not officially des-
 14 ignated as waste, it is included as part of DOE's mixed waste inventory in the "180-day report" mandated by the *Fed-*
 15 *eral Facility Compliance Act of 1992* (FFCA, 1992). Thus, while in storage, high-level waste and spent fuel would
 16 appear to be subject to the *Resource, Conservation, and Recovery Act of 1976* (RCRA) and subsequent amendments.
 17
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 19

20 Whether the mixed waste is subject to RCRA after disposal is not clear. The statement in the Energy Policy Act
 21 that the new EPA standards "shall be the only such standards that apply to the Yucca Mountain Site" would encourage
 22 the idea that compliance with RCRA and other standards (such as the Clean Water Act, 1977) *in addition* to the new
 23 EPA standard will not be necessary. The 1994 PA assumed this intent and thus did not consider RCRA or other such
 24 standards as a primary control with regard to nuclear waste disposal. However, in the analysis, several nonsorbed,
 25 long-lived radionuclides were transported in gas and liquid. These results can be used to evaluate maximum concen-
 26 trations of hazardous chemicals at the boundary of the disposal system.
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30 Additional discussion of hazardous waste materials is provided in Chapter 2.
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34 1.3 Organization and Mechanics of the Performance Assessment

35 The primary means of determining whether a waste is acceptable for inclusion as part of a geologic disposal sys-
 36 tem is a performance assessment (PA). The term performance assessment is generally defined as the process of
 37 assessing whether a *system* meets a set of *performance criteria* (Rechard, In preparation, p. 1-1).^{*} For a geologic dis-
 38 posal system, the *performance criteria* are various long-term (10,000 yr and longer) environmental metrics specified
 39 in government regulations. For assessment of the long-term consequences of a geologic disposal system, the tech-
 40 nique used is computer simulation; thus, the *system* for the performance assessment is a computational *model* that
 41 represents the geologic disposal system, not the system itself. Consequently, a performance assessment for evaluat-
 42 ing geologic disposal of nuclear waste is intimately tied to the general scientific processes of modeling as is evident in
 43 the next two sections.
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50 1.3.1 Six Steps of a Performance Assessment

51 For discussion, the organization and mechanics of the Sandia process for assessing the compliance of the dis-
 52 posal system with 40 CFR 191 (especially the Containment Requirements in §191.13) and other long-term (10,000 yr
 53 in U.S.) regulations can be conveniently categorized into six general steps (Figure 1-1). The six tasks are as follows
 54 (Rechard, 1989):
 55
 56
 57
 58
 59

60 ^{*} This more general definition of a performance assessment is used herein; however, the 40 CFR 191 regulation defines a performance assess-
 61 ment as "an analysis that (1) identifies the processes and events that might affect the disposal system, (2) examines the effects of these pro-
 62 cesses and events on the performance of the disposal system, and (3) estimates the cumulative releases of radionuclides, considering the
 63 associated uncertainties, caused by all significant processes and events." In essence, the definition of performance assessment is tied specifi-
 64 cally to one particular performance metric, the evaluation of cumulative releases of radionuclides. Also, the phrase "considering the associ-
 65 ated uncertainties" implies the use of a stochastic simulation as the evaluation technique instead of estimating a variety of performance
 66 metrics.

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Figure 1-1. Sandia's method for conducting INEL Performance Assessment calculations involves six general tasks (after Rechar, 1989, Figure 3.1). This report is organized around these tasks. Components of the tasks shown with dashed lines were not performed in this performance assessment. Also, note that iterative refinements are not shown but should occur in the future.

1. Collection of data on (a) spent fuel and high-level waste, (b) geology and hydrology near the site and (c) facility design to characterize the disposal system and regional area (system characterization); first phase in conceptual model development.
2. Identification of features and agents (i.e., the continuous phenomena, sometimes called processes, and short-term phenomena, called events) of the disposal system whereby radionuclides might be released to the accessible environment, and selection of a set of mutually exclusive scenarios (from known features, events, and processes) (scenario development); second phase in conceptual model development (i.e., the selection of what to model).
3. Development and execution of probability models that quantify the uncertainty in model parameters and predict the likelihood of the scenarios (probability modeling),
4. Development and execution of consequence models to predict the amount of radionuclide release to the accessible environment, including evaluating the uncertainties associated with the predictions (consequence modeling),
5. Comparison of the predicted releases and doses with government regulations (regulatory assessment),
6. Evaluation of the important model parameters that most influence the calculated results (sensitivity/uncertainty analysis).

The remainder of this Introduction and the report itself are organized according to these general tasks.[†]

1.3.2 Results of Six Steps in Performance Assessment

Each step generates results, which are reviewed and used in subsequent steps. Figure 1-2 is a simplified chart of the results of each step (Rechard, In preparation).

1. *Parameter space.* The results of the first step are used to determine the parameter space for the conceptual model, $D = \{x_1, x_2, \dots, x_{nP}\}$ where nP is the total number of parameters of the disposal system. The parameters are subdivided into three disjoint subsets: uncertain parameters typically classified as stochastic variables and thus often studied through scenarios (e.g., event and feature parameters), uncertain parameters typically expressed as a random variable (e.g., material property parameters), and parameters selected to be fixed or varied one at a time (e.g., model domain parameters, physical constants).
2. *Scenarios.* The result of this step is a description of the state of the uncertain parameters (being studied through scenarios) that define a particular condition of the disposal system (e.g., intrusion, no intrusion).
3. *Probability Models.* This step creates two types of results: models that evaluate the probability of the scenario occurring and distributions that express the uncertainty of parameters. At this step, the parameter space for the performance assessment model can be identified, D' , which usually contains only subtle modifications to the original parameter space (see 1, above).
4. *Consequences.* The results of this step are the consequences of the simulations. Monte Carlo simulations are used to propagate the parameter uncertainty through the model and require many simulations.

[†] These six steps can also describe a probabilistic risk assessment (PRA) which, like a performance assessment, is a stochastic simulation (see Chapter 3, Overview of PA Methodology). The main difference between the two assessments is that the term, "PRA," is, in general, associated with only engineered facilities over short geologic time scales, while the term, "PA," is associated with a combination of natural and engineered systems over long geologic time scales.

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Figure 1-2. Depiction of the results of six steps in a performance assessment.

5. *Analysis.* The results of the analysis are usually presented as a mean or a family of complementary cumulative distribution functions (CCDF). This summary is used to compare the generated consequence of each scenario and its corresponding probability with regulatory criteria.
6. *Sensitivity/Uncertainty Analysis.* Because a summary result, such as a CCDF, can obscure certain aspects of the results, the final step generates results that illustrate the sensitivity of the consequences to uncertain parameters.

Further information on the general PA methodology is found in Chapter 3.

1.4 System Characterization

System characterization is the first phase in conceptual model development. In this phase, the physical systems such as the waste, its treatment options, the geologic repositories, and the backfill and seals, are defined and represented in the consequence model.

1.4.1 Waste Containment System Terminology

As used in 40 CFR 191, a radioactive waste containment system includes three major subsystems (institutional controls, geologic barriers, and engineered barriers) and their corresponding major components (Figure 1-3) (see also Figure 2-2 in Chapter 2). The first subsystem, institutional controls, consists of components such as legal ownership of the land and resources by the U.S. Government, fencing and signs around the property, permanent markers, public records and archives, and other methods of preserving knowledge about the disposal system (Trauth et al., 1993; Rechard et al., 1993). Effects of this subsystem are not included in the performance of the tuff repository.

The second subsystem, geologic barriers, is limited to the lithosphere up to the ground surface and no more than 5 km (~3 mi) from the outer boundary of waste-emplacement rooms and drifts. A boundary of 2.4 km was used for the geologic barrier for the 1994 PA. (The land-withdrawal boundary for the salt repository was 2.4 km and was used for the 1993 PA.)

The physical features of the repository (e.g., design of the repository, waste form, waste parcel, and backfill) are components of the third subsystem, engineered barriers. For purposes of discussion, the components of the engineered barrier system are grouped into two subsystems: the waste parcel and the repository. In this report, the waste parcel is defined as the waste form, waste container, and two overpack containers. (The 1993 PA also included internal backfill in the waste parcel.) The term waste emplacement package signifies the waste parcel in the drillhole; when backfill-buffer is used between the waste parcel and the host rock, the backfill-buffer is considered part of the waste emplacement package. (As discussed later, this performance assessment assumes an air gap instead of backfill-buffer.) The repository includes the waste disposal rooms, access drifts, and access shafts, but does *not* include either the above-ground facilities or the undisturbed host rock. (Note that this term differs from the definition in 10 CFR 60 for "geologic repository," which is described as the disposal system and the current surface facilities.)

The disposal system, as defined by 40 CFR 191, includes only the geologic and engineered barrier subsystems. As part of the 1994 PA, analysts have investigated how the disposal system behaves, assuming specific situations (i.e., combinations of features, events, and processes) that represent possible future conditions at the repository. Depending on the situation, different parts of the engineered and geologic barrier subsystems are assembled into a system that can be modeled. These modeling systems are described below in Section 1.7, "Consequence Modeling," and in Chapters 9 through 14.

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Figure 1-3. Subsystems and components of a radioactive waste containment system. The disposal system, as defined in 40 CFR 191, comprises the geologic and engineered subsystems of the waste containment system (after Rechard et al., 1990, Figure 1-10). Herein, the engineered barrier subsystem is discussed as a waste parcel and a repository.

1.4.2 Waste Parcel Description

As described above, the waste parcel includes the waste form (e.g., graphite spent nuclear fuel), the waste handling container, and any disposal containers (overpacks). (Herein, waste refers to the contents of a nuclear waste container such as spent nuclear fuel rods, brackets, and hardware with the exception of any filler (internal backfill) packed inside the waste container.) In this section, the types of waste being modeled are described; the inventory of radionuclides and hazardous constituents found in the waste is provided; the options for treating the waste before disposal are defined and finally, the physical characteristics of the waste containers are detailed. For the 1994 PA, a source term model was developed specifically to accommodate the diverse characteristics of the fuel, including radionuclides residing in 10 different matrices and up to 8 nested layers of semiprotective material; the model is described in Section 1.7 and Chapter 11.

Waste Types. Both spent nuclear fuel and high-level waste are being considered in the 1994 PA. Five types or categories of spent nuclear fuel are included in this performance assessment: four from INEL and one from Hanford. The four waste categories from INEL are representative of over 90 types of fuels currently stored there. Over 90% by weight of the projected fuels have been shipped to INEL for storage, with the balance of these fuels located at their generation site, such as the Fort St. Vrain reactor in Colorado.

The spent fuels under study are graphite spent nuclear fuel, highly enriched uranium spent fuel, robust highly enriched uranium spent fuel, low enriched uranium spent fuel, and weapons production fuel. Specific fuels that are being modeled to represent the spent fuels are from Fort St. Vrain, graphite; Advanced Test Reactor (ATR), highly enriched; Shippingport, robust highly enriched; pressurized water reactor (PWR), low enriched; and N-Reactor, weapons production.

The graphite spent nuclear fuel is grouped separately from the other spent fuel not only because its characteristics differ from other fuels but also to maintain continuity with the 1993 PA. The physical characteristics are represented by the Fort St. Vrain fuel, but the radionuclide inventory includes fuel also from the Peach Bottom 1 reactor in Pennsylvania.

The ATR spent fuel was selected to represent the physical characteristics of HEU fuel because it makes up a good portion of the HEU fuel at INEL and is also one of the most chemically reactive fuels stored there. The inventory from other fuels is included.

The Shippingport HEU fuel, which was not considered in the 1993 PA, is included because it is considered to be one of the most robust fuels in the harsh environment of a repository. The inventory of the fuel from Navy propulsion reactors is included with this waste type.

The spent fuel from pressurized water reactors (PWR) for research is similar to commercial fuel, but has a lower burnup. The radionuclide inventory from commercial PWR fuel stored at INEL is also included with this waste type.

The N-Reactor fuel is not currently stored at INEL—it is held at the Hanford reservation in Washington state. However, it is included in the 1994 PA because it represents ~80% by MTHM of the current spent fuel inventory owned by the DOE and a large portion of the spent fuel inventory by other measures as well (refer to next section, Inventory).

The INEL high-level waste being modeled primarily originates with spent fuel that has been accepted for interim storage and reprocessing since 1953 by DOE at the Idaho Chemical Processing Plant (referred to herein as the Chem Plant). Although recycling of the spent fuel was discontinued in 1992, its purpose was to recover uranium, krypton, and other resources. During this process, both high-level and low-level liquid wastes were produced. The high-level liquid waste was heated to form oxides and fluorides, collectively called calcine. Sodium-bearing liquid waste from decontamination of facilities and other sources was also produced; this waste was also blended with the high-level liquid waste to form calcine because it was difficult to calcine the sodium-bearing liquid waste directly. Because it is generated from decontamination of facilities, the sodium-bearing liquid is not classified as high-level waste. However, its activity is greater than Class C low-level waste (Ermold et al., 1993), and is managed as high-level waste at

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the Chem Plant; hence, it is included here with the high-level waste inventory. For the 1994 PA, the calcined waste is modeled primarily as a glass-ceramic waste form. However, note that in the Simple PA, described in Section 1.5.2, the calcine is also modeled as a borosilicate glass waste form and a loose, granular solid, for purposes of comparison with the 1993 PA.

Like the 1993 PA, each waste type under study was evaluated individually (Simple PA) and also studied in combination as a disposal group (Complex PA). The purpose of grouping the wastes was to more realistically evaluate the behavior of the waste in a moderately sized repository. Since it is clearly not cost effective to build a repository for just the fuel under study (i.e., the spent fuel and high-level waste stored at INEL and the N-Reactor fuel from Hanford), when the waste types were studied in combination, high-level waste from three DOE sites was added to the hypothetical repository to illustrate what a more realistic repository would contain. The DOE high-level waste was also used for comparison with the behavior of the INEL and Hanford wastes. The inventory from the DOE sites includes high-level waste immobilized in borosilicate glass from (1) the Savannah River Plant (SRP), produced at the Defense Waste Processing Facility (DWPF) near Aiken, SC; "Savannah River"; (2) Hanford Waste Vitrification Plant (HWVP), Hanford, WA, "Hanford"; and (3) West Valley Demonstration Project (WVDP), West Valley, NY, "West Valley", formally a demonstration plant for reprocessing commercial spent fuel.

In summary, seven waste types are modeled in 11 unique waste parcels. Three waste parcels contain the calcine waste from INEL, each processed differently, and another three contain the high-level waste from three DOE sites. The waste types in each parcel are as follows:

Spent Nuclear Fuel:

1. Graphite spent nuclear fuel, represented by fuel from Fort St. Vrain reactor in Colorado.
2. Highly enriched uranium (HEU) fuels, i.e., fuel originally with over 20% by mass fissile ^{235}U isotope; represented by Advanced Test Reactor (ATR) fuel.
3. Robust HEU fuel, represented by Shippingport fuel (a developmental fuel from the Light Water Breeder Reactor research program, Shippingport, Pennsylvania).
4. Low enriched uranium (LEU) fuel, i.e., fuel originally with less than 20% by mass fissile ^{235}U isotope; represented by commercial pressurized water reactor (PWR) fuel.
5. Weapons production fuel, represented by N-Reactor fuel (from Hanford, Washington).

High-Level Waste:

6. Calcine, immobilized at high temperature to form a glass-ceramic by using a Hot Isostatic Press (HIP) (from INEL); HIP is a process of mixing radionuclides into a glass-ceramic frit, the density of which increases from the high temperature and the moderate pressure in a metal container as the mixture solidifies.
7. Calcine, immobilized at high temperature by vitrification to form a borosilicate glass (from INEL).
8. Calcine, packaged loose as granular solid (from INEL).
- 9-11. High-level waste sludge immobilized by vitrification from three DOE sites: Savannah River, Hanford, and West Valley.

Inventory. This section provides information about the radionuclides contained in the waste, their activity, and the mass of the waste.

Radionuclides. The decay chains for the spent fuel and high-level waste considered in the 1994 PA contain 156 radionuclides. Most are short-lived. The initial inventory considered in the year 2030 was 63 radionuclides (Appendix A). These 63 radionuclides are modeled in the cuttings model and for determining the amount of heat generated by each container. Thirty-two radionuclides are modeled in the source term submodel for releases from groundwater. (The models are described in Section 1.7, Consequence Modeling.) The distribution of radionuclides differs for each waste type and is described in Chapter 4 and Appendix A.

Activities and Masses. The activity of the spent fuel stored at INEL is expected to total about 2.3×10^8 Ci in year 2030. The spent fuel from Shippingport makes up about 77% of the activity, but its mass of 350 MTHM[‡] represents only about 13% of the total mass of spent fuel stored by all DOE facilities (Table 1-2; Figure 1-4). The activity of the

[‡] MTHM is the mass of all isotopes of uranium, plutonium, and thorium before irradiation in a reactor, expressed in metric tons (1000 kg).

Table 1-2. Total Inventory for Hypothetical Repository (see Chapter 4)

	Waste Volume* (m ³)	Mass		Activity in 2030 (Ci)
		(MT)	(MTHM**)	
Idaho National Engineering Laboratory				
Spent Fuel				
Graphite (Fort St. Vrain)	293	352	28	4.23 × 10 ⁶
HEU (ATR)	315	63	72	4.09 × 10 ⁷
Robust HEU (Shippingport)	931	3780	110	1.74 × 10 ⁸
LEU (PWR)	167	250	162	2.07 × 10 ⁷
High-Level Waste	4250	14892	320	1.50 × 10 ⁷
Hanford Reservation				
Weapons Production Spent Fuel (N-Reactor)	205	2300	2100	3.03 × 10 ⁷
DOE Facilities***				
High-Level Waste (borosilicate glass)	4727	12633	9268	1.71 × 10 ⁹
Totals	10888	34270	12060	1.12 × 10 ⁹

* The waste volume and gross mass changes with treatment. These values represent the current volumes and masses of the waste. Chapter 4 and Appendix A provide more details.

** Metric tons of heavy metal, an important unit for regulations, represents the original mass of all isotopes of uranium, plutonium, and thorium present in the fuel before being placed in a reactor. However, calculating the equivalent mass of heavy metal from the current volume of liquid high-level waste is subject to much uncertainty in comparison to the estimate for spent fuel. For this performance assessment, we used the methods defined in 40 CFR 191, as explained in Appendix C of this report. However, these methods can yield substantially different values if, as assumed in the mission plan for Yucca Mountain, each canister of high-level waste shipped to the repository is assumed to contain 0.5 MTHM (U.S. DOE, 1988b).

*** High-level waste inventory is from double-shelled tanks located at Hanford; high-level waste inventory from single-shelled tanks at Hanford is not included.

N-Reactor spent fuel stored at Hanford is expected to total about 3.0×10^7 Ci, with 2100 MTHM (Table 1-2). The heavy metal mass from N-Reactor fuel represents about 80% of the heavy metal mass of spent fuel stored by DOE facilities and about 82% of the uranium mass (MTU) (Figure 1-4). The activity of the high-level waste at INEL is expected to total about 4.7×10^6 Ci in 2030, with about 320 MTHM equivalent units (as calculated by the most conservative method described in Appendix A of 40 CFR 191).

Together, the INEL spent fuel and high-level waste, the N-Reactor spent fuel, and the DOE site waste total 12,060 MTHM. This total inventory still does not represent all of the DOE spent fuel and high-level waste, e.g., decontamination and site cleanup at DOE facilities could result in more high-level waste. For instance, the high-level waste inventory includes the waste form from only the double-shelled tanks, because the inventory from the single-shelled tanks was not readily available for this study. Also, the dismantling of U.S. nuclear weapons will result in more than 50 MT of plutonium and hundreds of megatons of highly enriched uranium (NAS, 1994, p. 1). However, the 12,060 MTHM is close to the 10,000 MTHM that was modeled in the 1993 PA, which is also the amount of spent fuel and high-level waste that was clearly identified and for which early plans for disposal were developed by DOE (e.g., U.S. DOE, 1985b, p. 1-10).

The combined volume and MTHM equivalent of the INEL spent fuel and high-level waste are 56% and 23%, respectively, of the total hypothetical repository (Table 1-2). In an actual repository, the addition of commercial waste, per the *Nuclear Waste Policy Act of 1982* (NWPA, 1983), would further decrease this percentage and reduce the influence of waste under study, making it more difficult to identify the behavior of the minimal waste treatment

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Figure 1-4. Mass (as of 1992) and volume of spent nuclear fuel (SNF) storage at DOE facilities. Spent fuel from INEL and Hanford are included in the 1994 PA. Only spent fuel from INEL was included in the 1993 PA. The values shown are based on data submitted to INEL for preparation of a draft Environmental Impact Statement (U.S. DOE, 1994); these values are more current (and slightly less) than those compiled in Appendix A, which were used in this report.

option described below.** The influence of high-level waste and spent fuel from the DOE defense complex on the overall performance of a repository filled with commercial spent fuel can be addressed in later studies.

Calculations were performed to estimate the inventory of gaseous fission products, using ORIGEN2 (see Chapter 10). ¹⁴C is of special concern because current requirements in 40 CFR 191 regarding the release of this moderately long-lived radionuclide are stringent. For the calculation, the principal source of ¹⁴C was assumed to be the neutron activation of nitrogen (¹⁴N), which is present in the fresh nuclear fuel as an impurity. However, for about 10% of the fuels, data regarding the amount of ¹⁴N were not available. Also, the ¹⁴N in the zirconium cladding that surrounds the fuel or in other metals of the fuel assembly was not considered. Hence, the estimate of ¹⁴C is slightly low.

Waste Treatment Options. For spent nuclear fuel, the treatment option modeled in the 1994 PA is disposal with either minimal or no treatment, which equates most closely to Option 1 in the 1993 PA. The spent fuel assemblies are packed reasonably tightly into the waste containers, which results in fewer containers than estimated in the draft Environmental Impact Statement for spent nuclear fuel management at INEL (U.S. DOE, 1994). The condition of the graphite spent fuel (Fort St. Vrain), robust highly enriched spent fuel (Shippingport), and low-enriched spent fuel (PWR fuel) is good enough that these wastes can be placed directly into handling containers for storage and eventual disposal. Some of the highly enriched spent fuel (aluminum-clad, uranium-metal ATR fuel) was damaged from corrosion during storage in water basins; some of the weapons production fuel (zircaloy-clad, uranium-metal N-Reactor fuel) was damaged routinely when ejected from the reactor core. The current plan for the ATR fuel is to dry the assemblies, arrest corrosion, and then place the assemblies into stainless steel sealed capsules. The capsules could then be placed in handling containers and into dry storage awaiting transport to a disposal system. Although some type of drying and stabilization will be required for the N-Reactor fuel, no final plans are available at this time.

** In DOE planning documents, the amount of DOE high-level waste proposed for the potential repository at Yucca Mountain, which has a proposed disposal capacity of 70,000 MTHM, was 7,000 MTHM (U.S. DOE, 1988b) and 10,000 MTHM (DOE, 1985a). Currently, no written policy exists that specifies the amount.

Hence, the assumption was made that only drying and stabilization were necessary before the fuel was placed in the handling container for storage and eventual disposal. The heat from oxidizing all the uranium metal in the N-Reactor fuel is about 1.34×10^{10} kJ. Although this amount is not minute, it is only one-tenth of the heat energy produced in one year by all the waste in the 12,060-MTHM repository and is not enough to significantly affect the calculations in the 1994 PA.

Three treatment options will be modeled for the calcined high-level waste from INEL: (1) glass-ceramic, (2) borosilicate glass, and (3) loose, granular solid. Glass-ceramic waste forms use various glass-forming additives and reactants to form the final product. This glass-ceramic product consists of an assemblage of crystalline phases bonded together by an intergranular amorphous (glass) phase. The final treatment process employs temperatures up to 1323 K (1050°C) and pressures ranging from 6.9×10^7 to 1.4×10^8 Pa in the HIP process. The advantage of the HIP process over borosilicate glass is improved volume reduction (higher waste loading), because fewer minerals without entrained radionuclides ("inerts") such as silica are formed. For borosilicate glass, the low calcine loading relative to the quantity of additives needed to make the borosilicate glass results in a significant volume increase. Although no leach test under simulated repository conditions has been run, standard leach rate testing has demonstrated slightly better results for the glass-ceramic; while leaching of radionuclides from the glass phase of the glass-ceramic is similar to borosilicate glass, leaching from the crystalline ceramic phase is slower. The different alteration rates for the two encapsulating matrices in the glass-ceramic are included in the source term submodel (see Chapter 11).

Only the borosilicate glass option is considered for the high-level waste (liquid, slurries, and solid) stored at Savannah River, Hanford, and West Valley.

Chapter 4, "Waste and Waste Parcel Description," and Appendices A and F provide details on such major characteristics as radionuclide inventory, volume solubility, and release of radionuclides from alteration of the encapsulating matrix for the minimally stabilized waste.

Characteristics of Waste Container. In the 1994 PA, waste containers include both the handling container and up to two disposal containers (overpacks). A disposal container is an outer container placed around the handling container that provides a specific function such as corrosion protection or corrosion allowance. (Except for one calculation set, overpacks were not modeled in the 1993 PA so that attention could be focused instead on the five waste treatment options.) The container modeled in the 1994 PA is based on the conceptual design for the Yucca Mountain Project, which is intended to meet the container requirements of 10 CFR 60, including a waste package that will last 300 to 1000 yr. The details of the containers and the internal "basket" that support the waste types are discussed in Chapter 4 and in Appendix F.

In general, three types of waste handling containers are being modeled in the 1994 PA: the 125-ton Multi-Purpose Canister (MPC) for horizontal emplacement, the 25-ton Legal Weight Truck (LWT) canister for vertical emplacement, and the DOE standard high-level waste canister (used for both vertical and horizontal emplacement). The material for all three handling containers is stainless steel type 304L. The thickness of the MPC is 25.4 mm; both the LWT container and the DOE standard container are 9.5 mm.

The waste canisters are placed in two disposal containers (overpacks): a 20-mm corrosion resistant overpack of Incoloy Alloy 825, which directly covers the handling container, and a 100-mm corrosion-allowance overpack of carbon steel^{††} (Figure 1-5).^{‡‡} (To evaluate the influence of the corrosion-resistant layer, a few calculations were run in

^{††} ASTM Type A-516, Grade 60, is assumed when "carbon steel" is referred to, throughout document.

^{‡‡} It should be noted that the current conceptual design for the Yucca Mountain Project does not consider the LWT. Also, the current plan for an outer containment barrier consists of a 100-mm corrosion-resistant layer of 70-30 Cupronickel alloy for the borosilicate glass waste form rather than carbon steel. This substitute layer was proposed because preliminary experiments indicated that silica in the glass showed higher solubilities in the presence of iron. However, the Cupronickel layer is replaced with the standard carbon steel layer in the 1994 PA, in large part so that a common basis of comparison can be maintained among the containers. Other factors that contributed to the decision were that the distribution range for the silica glass dissolution is already four orders of magnitude; the increase in solubility of the glass could not be determined without further evaluation of data; and, finally, the understanding that iron has a potentially beneficial effect in that it can make the chemical environment inside the container reducing for a very long time, thus lowering the solubility of Np and some other actinides. It was beyond the scope of the 1994 PA to examine these competing effects.

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25-Ton Legal Weight Truck (LWT) Canister
with Disposal Overpack Containers

"Standard" Canister for DOE
HLW (Container Placed in Disposal
Overpack Composed of Same
Layers as LWT)

(a) Vertical Emplacement

125-Ton Multi-Purpose Canister (MPC) with Disposal Overpack Containers

(b) Horizontal Emplacement

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Figure 1-5. Legal Weight Truck (LWT) canister and Multi-Purpose Canister (MPC) with disposal overpack containers used in 1994 PA.

which the 20-mm layer was assumed to be present but not protective against corrosion.) The MPC would be shipped by rail; the LWT could be transported by truck.***

Spent Fuel Handling Containers. Spent fuels with minimal conditioning were assumed to be placed directly into the 125-ton MPCs or the 25-ton LWT canisters and placed in the repository. The number of spent fuel assemblies per handling container was based on the maximum number of unmodified (e.g., not compacted) assemblies that could fit into the container without difficulty. A borated stainless steel frame was used to support the fuel and prevent critical conditions during loading of the containers under water; the frame's size and shape varied by fuel type. After disposal, at elevated temperatures and in the presence of moisture, both the frame and the fuel could rapidly corrode. The preferential removal of either the boron-chromium crystals or the uranium was examined and is described in Chapter 10 under the discussion of the potential for critical conditions.

High-Level Waste Containers. For horizontal emplacement, handling containers of both INEL and DOE high-level waste will be placed inside MPCs and then into disposal containers (overpacks).††† For vertical emplacement, handling containers of calcine high-level waste from INEL and DOE borosilicate glass waste are placed in disposal containers (overpacks) of Incoloy Alloy 825 and carbon steel, and then into boreholes.

1.4.3 Geologic Barrier Characterization

Tuff, granite, and salt are rock types that have been under study as geologic barriers for disposal of spent nuclear fuel and high-level waste. In the 1994 PA, tuff — formed from welding of hot volcanic ash — is being modeled. The purpose of modeling tuff is to compare its results to those from the generic salt and granite repositories, which were modeled in 1993, and to study the effects of disposing minimally treated spent fuel and high-level waste in geologic media similar to the Yucca Mountain Project, which is currently under consideration for disposal of commercial spent fuel and defense-related high-level waste in the U.S.

The general technical criterion for a geologic barrier is an ability to physically isolate radionuclides from the biosphere. In addition, the barrier should provide a measure of physical and chemical stability. Advantages of tuff as a geologic barrier are that it is located relatively near the surface in areas remote from human populations; contains layers of zeolites, which absorb radionuclides; and includes groundwater flow that is saturated with silica, which reduces the solubility of radionuclides. Also, because the tuff is located in a desert, the repository can be placed in an unsaturated zone, which limits the amount of water that can degrade containers and transport radionuclides to the accessible environment.

Geologic units have been mapped at Yucca Mountain, but some of the tuff stratigraphy cannot be simplified with confidence since data are preliminary. The hydrologic units for the 1994 PA are idealized as a series of constant thickness tuffs ("pancakes") tilted at 4.6° from the horizontal. These units consist of consecutive layers of tuff with degrees of welding (i.e., porosity) that were similar. Although the modeling units roughly correspond to the formal geologic stratigraphy, some units contain only a portion of a formation member or overlap several formation members. The thicknesses of the units are based on data from two wells near Yucca Mountain, USW G-3 and USW G-4. The repository is assumed to be located at a depth of about 300 m below the surface in the Topopah Spring member of the Paintbrush Tuff Formation, which is in the unsaturated zone. An aquifer lies about 300 m below the repository (Figure 1-6). The stratigraphy is more thoroughly described in Chapter 5, "Geologic Barrier."

Characteristics of the hydrologic modeling units strongly influence how well the waste is contained. Important hydrologic characteristics are the flow-related properties, such as permeability and porosity; local and regional groundwater percolation, which is used to assess the degradation of containers and transport of waste from the repository.

*** When it is important that details about a waste package be distinguished, then this report specifically refers to the handling container (i.e., the MPC or LWT) and the two overpack disposal containers. However, when only the size or orientation of the waste is being discussed, the complete container is referred to simply as either the MPC or LWT.

††† The current conceptual design for waste containers for Yucca Mountain Project places four DOE canisters directly into the disposal containers (overpacks), adding top and bottom spacers, instead of first placing them into an MPC.

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Figure 1-6. Simplified cross-section used in two-dimensional simulations. The eleven hydrologic modeling layers include groups of consecutive geologic layers that have similar porosity (i.e., welded or nonwelded).

itory; and thermal properties, which are affected by the radioactive waste since it generates heat for the first few hundred years. Because the emphasis of this performance assessment is the behavior of the waste, many parameters for the geologic site characterization data were not varied. The Complex PA uses a slightly more complicated two-dimensional representation of the tuff disposal system than was used in TSPA-1993 for Yucca Mountain (Wilson et al., 1994), but most of the interpreted data on characteristics of the tuff presented in TSPA-1993 are used in this performance assessment without reevaluation. For example, although the TSw unit of the Topopah Sprint unit could be further divided into two units based on porosity and thermal conductivity properties, TSw was kept as a single unit to remain consistent with the TSPA-1993 data. The difference could influence temperature profiles, but the use of data other than those available for TSPA-1993 was beyond the scope of the 1994 PA.

Related to the geologic barrier is climate change, an agent that acts upon the unsaturated tuff and which has been shown to be important to waste containment because it can enhance infiltration and thus percolation through the unsaturated zone (see, for example, Barnard et al., 1992; Wilson et al., 1994). The possible variation in infiltration rates from climate change is modeled in the 1994 PA, although it was not included in the 1993 PA because the influence on the saturated aquifer above the salt repository was thought to be minor (see WIPP PA Division, 1991c) and the flow rates through the granite repository were already quite large. The 1994 model is meant only to simulate variation of infiltration, not to predict when changes in infiltration will occur.^{†††} The climate variation is modeled with a sinusoidal increase of infiltration. The three important parameters of the sine function (minimum infiltration, maximum infiltration, and period) were sampled from distributions with a mean of 0.5 mm/yr (interglacial climate) to a mean of 10 mm/yr (ice age climate), with a mean period of 100,000 yr, as used in TSPA-1993. The mean infiltration of 10 mm/yr for the wet climate is uncertain and does not explicitly include climate perturbations from anthropogenic sources, e.g., greenhouse gases, but is considered conservative, especially because the area would remain in the rain

^{†††} The climate variation models for the performance assessment of the Waste Isolation Pilot Plant perform a similar function (Swift, 1993).

shadow of the Sierra Nevada range. In addition, a focus (or concentration) factor was used to represent saturation of a small portion of the tuff that lies directly below a concentrated area of rainfall, which is within the overall range of rainfall. In the Simple PA (described in Section 1.5.2, Calculation Design), the sinusoidal increase was simplified by using steady-state flow with an infiltration equal to the 10,000-yr average of the sinusoidal function. Also, no focus factor for the rainfall was used because the mathematical model for the Simple PA is one-dimensional. Chapter 5 provides additional assumptions regarding climate variation.

1.4.4 Repository Design

The engineered barriers consist of design elements that are intended to isolate the waste from the accessible environment. Components of the engineered barriers that are specific to the repository include (1) the subsurface facility layout, (2) the design for waste emplacement, and (3) specially placed backfill (a subset of which is often called a "seal") in the drifts and ramps. These concepts are more thoroughly described in Chapter 6, Repository Design. Two other design components are the waste form itself and the containers; these were discussed in Section 1.4.2, Waste Parcel Description.

Because many of the precise details of the repository—such as the need for ramps or ventilation, and the size of the operational area—depend more on the operational phase of the repository than behavior after closure, the discussion below and in Chapter 6 highlights only the dimensions considered pertinent to post-closure behavior, such as the minimum spacing of containers and rooms.

Subsurface Facilities. The disposal region of the repository was sized to accommodate 12,060 MTHM**** of spent fuel or equivalent high-level waste based on the number of waste parcels from INEL, Savannah River, Hanford, and West Valley (as described in Section 1.4.2). No other waste is included in the repository. The mine design for both vertical and horizontal emplacement is a room and pillar configuration, with the entire repository consisting of long rooms ("tunnels"). The rooms are surrounded and connected by access drifts, 7.65 m in diameter, which lead to ramps that connect to the surface (Figure 1-7). A tunnel boring machine is assumed for excavation of the rooms and drifts because it is the preferred mining scheme for the Yucca Mountain Project (TRW, 1993a).

Waste Placement in Repository. In addition to size, design features of the repository that can affect its long-term performance are the waste orientation and the spacing of waste parcels and rooms.

Orientation of Waste Parcels. For this performance assessment, two orientations for placement of waste parcels are considered: vertical emplacement in bored holes in disposal room floors and horizontal emplacement within the rooms. Vertical emplacement corresponds to the orientation modeled in the 1993 PA and to early conceptual designs for waste emplacement in the U.S. and internationally (e.g., U.S. DOE, 1988a). Because of concerns regarding waste handling and accompanying radiation exposure to humans, alternative orientations are being considered. The technical baseline design for the Yucca Mountain Project as of February, 1994, is horizontal emplacement, in which a limited number of large containers would be transported by rail both to and within the repository. The waste parcels, such as the 125-ton MPC, would be parked in the rooms for disposal.

Spacing of Waste Parcels and Rooms. Three factors potentially affect the spacing of waste parcels within the rooms and the distance between rooms: (1) thermal limits placed on the waste form and/or adjacent host rock, (2) ability to bore closely spaced boreholes and/or tunnel closely spaced rooms, and (3) potential for neutron interaction between containers, which would enhance the possibility of a critical condition. The controlling factors in the 1994 PA are considered to be the first and second factors (see also Chapter 6).

For *horizontal emplacement*, the 1994 PA had a thermal design goal of reaching as high an areal power density (ratio of power to area) as possible with the relatively cool DOE spent nuclear fuel and high-level waste. The goal

**** By comparison, the proposed size of the Swedish repository is about 7800 MTHM (SKB, 1992a, p. iv); the amount of waste stored in dry casks or pools at the 111 reactors in the U.S. in 1990 was about 21,500 MTHM (BRWM, 1992, p. 4); and the entire Yucca Mountain repository may store no more than 70,000 MTHM until a second repository is licensed (NWP, 1983, Section 114).

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Figure 1-7. Hypothetical repository setting and design.

was based on continuing studies by the Yucca Mountain Project to actively consider a high areal power density to determine whether any desirable effects are encountered, such as drying out the host rock for hundreds of years.

In pursuit of this goal, the MPCs are modeled as remaining on the underground rail transportation and placed end-to-end without spacing. Neutron interaction is expected to be minimal because of the large amount of metal present in the ends of the waste containers. (These and other criticality considerations are presented in Section 1.7.)

Two thermal limits are considered in the horizontal emplacement design for the Complex PA: (1) a maximum centerline temperature in a waste parcel to prevent excessive failures of fuel cladding and (2) a host rock/waste parcel interface temperature below 200°C to prevent undesirable thermal stresses around the room. The maximum centerline temperature was 350°C for most fuels, and 200°C for the aluminum-clad ATR fuel, which represents the highly enriched spent fuel. A third thermal limit, which was not designed into the repository but is evaluated in the results, is maintaining a temperature below 115°C at the interface of two hydrologic modeling units, TS_{wv} and CH_n (MacDougall et al., 1987b) (see Figure 1-6). This limit was originally proposed to prevent alteration of zeolites in the hydrologic modeling unit, CH_{nz}, which is directly below CH_n; alteration of zeolites may reduce their ability to sorb radionuclides. However, the importance of this thin layer has never been evaluated, so its potential for influencing radionuclide sorption was not considered during repository design. These thermal limits were considered only in the Complex PA, in which a repository with a mix of waste was evaluated. The Simple PA, which evaluated only one waste type at a time, adjusted the quantity (MTHM) of the fuel, the total power output of the fuel, and the spacing of the containers so that for most individual fuels the power density remained at the same level as in the Complex PA. However, the Simple PA did not consider the two thermal limits; the centerline temperature limit was exceeded by 20°C for ATR spent fuel, and the limit for the host rock/waste parcel interface was exceeded by 80°C for the Hanford borosilicate glass waste.

Rooms were spaced with the constraint that the pillar that separates the rooms be no less than the width of the room diameter. For horizontal emplacement, a 4.3-m-dia room was considered adequate, and thus a 4.3-m spacing was modeled. Although the ability to tunnel rooms this close together was not examined in detail, it appeared plausible.

The combination of the end-to-end spacing of the MPCs and the room spacing of 4.3 m resulted in an areal power density of 23.5 W/m² in the year 2030. This value represents the maximum areal power density that could be realistically obtained with the assumed mix of DOE spent nuclear fuel and high-level waste. The resulting enclosed area of the disposal region is 0.288 km² with about 42% of the volume removed (extraction ratio of 42%). By way of comparison, the Yucca Mountain Project has considered power densities as high as 28.2 W/m².

For *vertical emplacement*, the design goal of the 1994 PA was to achieve an areal power density of 14.1 W/m² (57 kW/acre),^{††††} which was an early conceptual design goal for the Yucca Mountain Project. For comparison with the 1993 PA, the design-basis areal power densities for waste disposal group 1 (minimal treatment) for the salt and granite disposal systems were 5.3 W/m² and 4.6 W/m², respectively.

The thermal constraint for vertical emplacement was a maximum temperature below boiling (~100°C) at the host rock/waste parcel interface to limit vaporization of groundwater. (This same constraint was considered in the 1993 PA.) The generally low temperatures produced by the DOE spent nuclear fuel and high-level waste permitted a minimum spacing of 2.6 m (8.5 ft) center-to-center in a compact hexagonal pattern in the room. The spacing calculated for neutron interaction fell below this range (see Appendix E); although the actual boring of holes was not examined in detail, the 2.6-m spacing appeared to be adequate.

For vertical emplacement, the rooms are 7.65 m wide to provide enough clearance to vertically bore the 5.5-m deep holes. The combination of the 2.6-m spacing of the boreholes and an areal power density of 14.1 W/m² in the year 2030 resulted in a 7.5-m spacing between rooms (slightly smaller than the width of the room itself). The result-

^{††††} This value was calculated as a design-basis areal power density, which uses an entire room and half the width of the pillars and access drifts around the room to define the area. However, because of the regular shape of the disposal area, this value is equivalent to a local areal power density, which is the area around a single container and half the distance to adjacent containers.

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ing enclosed area of the disposal region is 0.247 km^2 , which is somewhat smaller than the horizontal emplacement scheme; however, the extraction ratio of 42% is the same.

Backfill. As used herein, backfill is the material that fills the excavated openings of the repository. Special categories of backfill include (a) seals for providing immediate sealing of access drifts and ramps and (b) backfill-buffer,^{††††} which is placed directly around the waste parcel. In the 1994 PA, only the ramps to the disposal area were assumed to be backfilled and effectively sealed.

Backfill was not used in the access drifts, rooms, or directly around the waste parcel for either the horizontal or vertical emplacement schemes. An air gap was selected in place of backfill because the trapped air in crushed-tuff backfill, which has a low thermal conductivity, would act as an insulator, thus increasing centerline temperatures. Also, the gap provides a capillary break, which does not eliminate dripping but does limit contact of water percolating through the matrix.

How the air gap around the waste parcel was modeled depends on modeling capabilities and intended effects, and was treated in several different ways. For the calculation of heat transport directly around the waste parcel (see also Section 1.5, Scenario Development), an analytic solution for radiative heat transfer through the air gap was used; potential vaporization of water was neglected. For the calculation of one-phase fluid flow, the porosity of the air gap was added to the fracture porosity and a continuum assumed between the waste parcel and the host rock. For the calculation of coupled two-phase flow and thermal calculations in the Complex PA, the porosity of the gap was added to the fracture porosity in the grid. Thus, the thermal calculations in the Complex PA did not consider radiative heat transfer through the gap but allowed for potential vaporization of the water. For the source term calculations, both intact air gaps and gaps filled with rubble from degradation of the tunnel over time were considered because (1) the presence of the rubble meant that, in addition to dripping, the matrix could have contact with water percolation, and (2) a diffusion pathway through the rubble was a potentially important release mechanism for radionuclides. The codes used in these models are briefly discussed in Section 1.7, Consequence Modeling. Specifics on how the air gap was modeled for the source term submodel are provided in Chapter 11.

1.5 Scenario^{*****} Development

Herein, scenario development is considered the second phase of conceptual model development (the first phase being system characterization, Section 1.4). Generally speaking, scenario development is the process of deciding what may happen to the disposal system in the future and how to model it. Although scenario development is not always a formal step of conceptual model development, it is useful to formalize the process for a large analysis such as a performance assessment of a tuff disposal system.

Scenario development consists of several steps:^{†††††}

1. Identifying the full scope (i.e., "universe") of features, events, and processes of the disposal system. (Events are short-term phenomena; processes, long-term phenomena.)
2. Selecting those features, events, and processes that might contribute to contaminants being released to the accessible environment and omitting those phenomena that can be eliminated because of either low probability, low consequence, or a previous agreement regarding acceptable style of calculations (e.g., guidance in Appendix B of 40 CFR 191).

^{††††}The term "backfill-buffer" is used to denote backfill placed around a waste parcel. The term was used in the report of the 1993 PA because backfill around a waste parcel in granite was expected to moderate the release of contaminants to the host rock.

^{*****}The various meanings of "scenario" are discussed in Chapter 3, "Overview of Performance Assessment"; the reader is advised to peruse at least Section 3.3.1 in order to understand the contexts in which "scenario" is used here.

^{†††††}In other documentation, the term scenario development is often synonymous with steps 1 through 3 only, because these three steps initially attracted greater attention than steps 4 and 5. In this report, however, scenario development includes not only the selection of the features, events, and processes, but also the incorporation of those components into the computational model.

3. Grouping features, events, and processes into summary scenarios.
4. Creating conceptual model(s) based on (a) the disposal system characterization and (b) the selected features, events, and processes.
5. Designing performance assessment calculations that incorporate the conceptual model(s).

As seen in these steps, many decisions are made during scenario development about what to include in the model. The actual decisions, however, are detailed in the discussions on system characterization, probability models, or consequence models. The sections below briefly describe the outcome of scenario development.

1.5.1 Identified and Selected Features, Events, Processes, and Summary Scenarios

The selected features, events, and processes were drawn largely from previous studies, e.g., TSPA-1993 (Wilson et al., 1994). However, a formal identification and selection procedure was used to verify the completeness and reasonableness of the selections (e.g., Rechard, Ed., 1993; Rechard, In preparation, p. 3-3). Chapter 7, "Scenario Development," includes results of this procedure; Appendix E contains scoping calculations that were performed in support of scenario development (i.e., preliminary performance assessment, criticality safety calculations, and detailed analysis of solubility of radionuclides in silica-saturated solutions).

Because the focus of the 1994 PA is the performance of minimally treated waste in a robust container, some combinations of events and features were not evaluated, e.g., volcanism was not considered based on results from a previous performance assessment (Wilson et al., 1994), which showed a probability of occurrence to be just above 10^{-4} in 10,000 yr in conjunction with insignificant releases. The basic features, events, and processes selected for modeling in this performance assessment are briefly summarized below.

Features. The basic features explored in the 1994 PA are (1) a point where precipitation collects at the surface; (2) a highly fractured, pancake stratigraphy; (3) a large unsaturated zone that holds a repository; (4) vertical and horizontal emplacement of waste containers; and (5) an underlying aquifer. The features are described in Section 1.4 and Chapters 5 and 6.

Event. The basic event explored in this performance assessment is human intrusion through exploratory drilling. The main effect of the drilled boreholes is to bring cuttings containing radionuclides directly to the surface. Like the 1993 PA for the granite disposal system, the fracture permeability of the tuff stratigraphy was assumed high enough that the additional fluid paths created by the drilled boreholes would not significantly enhance fluid movement and radionuclide transport.

Processes. Basic processes are explored for the geologic barrier, waste form, waste container, and repository.

- *Geologic Barrier.* Processes considered are two-phase flow and heat conduction with possible phase change in a fractured, porous matrix, large degrees of sorption of selected radionuclides on tuff, and infiltration variations from climate change, with amount focused on center of the repository.
- *Waste Form.* The process considered is control of radionuclide release by solubility; matrix alteration or immediate release of some radionuclides in gaps and grain boundaries of spent fuel; and degradation of cladding and matrix containing radionuclides (except for fuel with initially failed cladding).
- *Waste Container.* Processes considered are gas consumption from several layers because of generalized oxic corrosion, radionuclide release through container controlled by localized corrosion, and diffusion through containers breach into the host rock.
- *Repository.* The process considered is radiative heat transfer through an air gap between container and host rock.

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The possibility of critical conditions (a waste form process) was considered as a separate scenario instead of being included as a coupled process within the consequence calculations. Although describing occurrences of a criticality and determining appropriate probabilities is difficult without accompanying consequence results, the separate scenario was considered the best option given the time constraints. Probabilities for the criticality event were evaluated with a fault tree, as described in Section 1.6. Some consequence calculations, as explained in Section 1.7, were performed that loosely coupled the phenomena to explore whether tightly coupled consequence calculations would be desirable in the future.

The incorporation of the features, events, and processes are discussed in Chapters 12 and 13, "Complex Consequence Modeling" and "Simple Consequence Modeling." The criticality calculations are described in Chapter 10, "Criticality Modeling."

1.5.2 Conceptual Models and Calculational Design

In addition to the identification and selection of features, events, and processes, other questions must be answered in designing the conceptual model and calculations:

1. How many parameters exist for which the ranges are not only sufficiently large to likely influence the results but also the sensitivity of the results to these parameters is of interest?
2. Should scenarios be discretized to obtain adequate coverage of various parameter categories (e.g., time of intrusion)?
3. How much simplification is acceptable for the features, events, and processes?
4. How much spatial and temporal detail is acceptable to run the calculations?

Item 1, identification of model parameters considered uncertain and the assignment of distributions, is described in Section 1.6 and Chapter 8. In this performance assessment, this parameter uncertainty is propagated through a Monte Carlo technique. Integration of mathematical equations through Monte Carlo techniques is discussed in Chapter 3, "PA Methodology Overview." Latin hypercube sampling is used to minimize the number of random samples needed in the Monte Carlo technique to adequately capture variability in the parameters and, thus, the number of simulations run in the consequence models (McKay et al., 1979; Iman and Conover, 1980).

Item 2, discretization of scenarios, is addressed only for the calculations of releases from cuttings, where time of intrusion is important. (In contrast, discretization can be important for scenarios in a repository in salt, where expected features and known processes do not appear to result in radionuclide release and release is initiated only through an external event such as human intrusion; see 1993 PA report [Rechard, Ed., 1993].)

Items 3 and 4, degree of simplification in the models, are addressed as they were in the 1993 PA by running two sets of modeling simplifications. The two levels of simplification were carried out in parallel so that the performance assessment could be completed in the time allotted. The purpose of two sets is to compare the results and explore the level of simplification possible for rapid response to future questions on alternative waste-treatment options. The first modeling approach is referred to as the "Simple PA" and the second as the "Complex PA." However, the terms simple and complex are relative only to each other; compared to many risk assessments, the Simple PA is quite detailed.

Simple PA. In the 1993 PA, the primary goal of a Simple PA was to use a level of simplification that allowed simulations to be set up quickly and geared toward fast run times, relative to the Complex PA. In the 1994 PA, the primary goal was to adopt models and methods similar to those used in TSPA-1993 (Wilson et al., 1994), which in turn had fast run times as a goal. Therefore, in the Simple PA, one waste type (e.g., graphite spent fuel) could be studied in the repository at a time, in addition to a mix of all waste types. Eleven single waste parcels were studied, including three INEL high-level waste forms: calcined waste in a glass-ceramic matrix, in borosilicate glass, and in loose granular form.

In the 1993 PA, the mathematical description of the conceptual model was made using a sophisticated set of ordinary differential equations to arrive at a lumped parameter model. In the 1994 PA, the method of modeling the phenomena was distinctly different. Specifically, the description of the natural phenomena consisted of (a) numerical solutions of one-dimensional versions of the mathematical model (e.g., the one-dimensional single-phase code, TOSPAC, was used [Dudley et al., 1989]), or (b) abstractions of results from detailed phenomenological models similar to those used in the Complex PA.^{****} The second method was used for evaluating transport of $^{14}\text{CO}_2$ in the unsaturated zone, where analytic curve fits to a two-dimensional analysis of gas movement driven by temperature increases were used, and for characterizing the transport results in the saturated zone obtained from the Complex PA. In the latter application of model abstraction, the path lengths and travel times of a neutrally buoyant particle were characterized as a distribution of path lengths and velocities, which were then placed in a one-dimensional single-phase analytic code for evaluating transport of nonsorbing, but decaying, radionuclides.

The consequence models used in the Simple PA are discussed in Chapter 13 and listed in Appendix G.

Complex PA. The Complex PA used detailed phenomenological simulation codes. The codes were based on mathematical models with potentially spatially distributed model parameters and used partial differential equations (PDEs) that were solved numerically on coarse grids. The regulatory performance criteria were evaluated directly from multiple execution of the simulation codes and thus provided a direct connection between the input data and the performance criteria. (When model abstraction is used to arrive at the simplification, as in this year's Simple PA, this connection can become somewhat obscure.)

The waste types, including all the spent fuels and the INEL high-level waste as a glass-ceramic, were studied as a group and with minimal treatment. In addition, high-level waste in borosilicate glass from three DOE sites (Savannah River, Hanford, and West Valley) was included. In the Complex PA, the waste was uniformly distributed in the repository.

The consequence models used in the Complex PA are discussed in Chapter 12 and listed in Appendix G.

1.6 Probability Modeling

For a performance assessment, two types of probability models are used. The first estimates the likelihood of uncertain parameter values by constructing distributions for imprecisely known model parameters. The second estimates the likelihood of the broad classes of the parameter space, called summary scenarios.

The first probability model, for imprecisely known parameters, is usually subjective but a probability model nonetheless. Because the purpose of this performance assessment is to examine minimal treatment of waste in a robust container, the primary criteria used to select which parameters to vary was the parameter's potential influence on waste form and container behavior. Thus, many parameters for the geologic barrier were kept constant. Although the subjective generation of probability distributions from system characterization data is a significant and time-consuming process for a repository that has been proposed, it can occur simultaneously with conceptual model development in a small integrated program such as this performance assessment. In keeping with this philosophy, the model parameters themselves are discussed in the chapters that characterize the system (Chapters 4, 5, 6, and 11). Chapter 8, Probability Modeling, provides a summary of the model parameters that were varied.

The second type of probability model is used to evaluate the probabilities of the scenarios. The probability of the selected scenario event—inadvertent intrusion into the repository by exploratory drilling—was evaluated with a homogenous Poisson probability model. The probability of the second selected scenario event—critical conditions occurring in a waste container—was evaluated in a fault tree with subjective estimates of the events leading to critical conditions (see Chapter 10 and Appendix B).

^{****}It was not the purpose of this report to examine the utility of using model abstraction to arrive at simple models. Rather, as previously stated, the goal was to approximate the techniques of TSPA-1993 (Wilson et al., 1994).

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As mentioned earlier, the occurrence of critical conditions developing in one or several containers containing highly enriched uranium was evaluated as a scenario instead of a general continuous process. Although this method was selected primarily due to time constraints, it offered the advantage of being able to focus solely on the occurrence of critical conditions. A disadvantage, however, was that without coupling to thermal and hydrologic fluid flow phenomena it was not possible to develop a knowledge base from which to estimate probabilities of events in the fault tree.

The probability models for the parameters and the human intrusion event are discussed in Chapter 8, "Probability Modeling." The criticality fault tree is discussed in Chapter 10 so that it could be included in the full discussion of the criticality calculations. The probabilities for the branches of the fault tree and the reasons for omitting some branches are discussed in Appendix B.

1.7 Consequence Modeling

A major portion of the performance assessment methodology consists of simulating the features, events, and processes to estimate the amount of contaminants released to the accessible environment, including propagating the uncertainties of model parameters to evaluate the uncertainties associated with the predictions. This step in the performance assessment process is referred to as consequence modeling. The model used for consequence modeling is actually a composite function of several models (Figure 1-8):

1. Cuttings release submodel (Chapter 9)
2. Criticality submodel (Chapter 10)

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Figure 1-8. Five categories of codes used for consequence modeling. The primary focus of the model was on phenomena related to the release of radionuclides near the waste container and bounding effects from critical conditions. Linkage of these codes is depicted in Chapter 7 and Appendix B.

3. Corrosion and source term submodel (Chapter 11)
4. Flow and transport submodels for Complex and Simple PAs (Chapters 12 and 13)
5. Biosphere transport submodel (Chapter 14).

Because the 1994 PA examined the acceptability of minimally treated waste forms, thus relying on the characteristics of the waste as is and the engineered design of the container, two efforts of prime importance were the modeling of phenomena related to the release of radionuclides near the container and the bounding of effects from critical conditions. Both efforts represent major undertakings, especially under the specified time constraints. More information about these efforts and the codes used is provided in the following sections.

1.7.1 Cuttings Release Modeling

For cuttings release, the WPRD code was used. WPRD, which is the same simplified version of CUTTINGS that was used in the 1993 PA, assumes that an exploratory drilling operation hits a waste container so that the entire contents of the container eventually move to the surface and, thus, the accessible environment. These releases are incorporated directly in the complementary cumulative distribution function (CCDF) for comparison with the EPA limiting line. The primary calculation determines the decay of the contents of the waste container up to the time of intrusion.

1.7.2 Criticality Modeling

Critical conditions in and around waste containers were studied with three types of models. Calculations with these models were performed in parallel. The first model is a refinement of the work performed in the 1993 PA on the minimum spacing necessary to eliminate most interactions of neutrons between adjacent containers. The second model attempted to bound the magnitude of potential energy in the repository by assuming a reactor at steady state for 10,000 yr. The third model examined the energy releases from a repository assuming a dynamic situation including processes that would stop the reaction, such as lack of water.

The second and third models, which were performed in parallel, pursued the problem of evaluating consequences should a critical condition develop within a container. The probability of these consequences was evaluated with a fault tree, as discussed in Section 1.6 and Appendix B. The importance of water to the occurrence of a critical condition must be emphasized. Not only must water be present but it must also bring about significant changes in the waste container and cause movement of uranium or neutron absorbers from the container. The current plan for loading the waste containers at DOE facilities is to load them underwater. Borated stainless steel is expected to be used for support structures inside the fully-flooded containers because boron is an excellent neutron absorber (i.e., "poison"); thus critical conditions would be prevented in the initial, fully-flooded configuration. Therefore to achieve a critical condition after disposal, either the fissile mass (^{235}U) would have to be removed from the vicinity of the boron, or the boron would have to wash from the container. However, either situation would require large amounts of water because of the low solubility of both the boron-chromium crystals from the corroded stainless steel support frame and the uranium from the fuel. The source term submodel, USATCONC (Chapter 11), monitors the inventory of the boron and uranium in the simulations to determine whether such changes occur; these results are presented in Chapter 15. The calculations discussed below and in Chapter 10 bound the consequences of the occurrence of a critical condition, based on the amount of water available to remove the boron (or move the uranium and precipitate it just outside the container) and thus produce conditions conducive to criticality.

Minimum Spacing. The calculations performed for the 1994 PA for vertical emplacement confirmed that spacing containers about 2 m apart, separated by intact tuff, was more than adequate to prevent significant interactions of neutrons. The calculations also indicated that because of numerous metal container lids on the MPC, containers could be placed end-to-end without an air gap for the horizontal emplacement without significantly increasing the neutron interactions between containers. These calculations are discussed in Appendix E. The neutral particle transport codes, MCNP (Breisemeister, 1986, 1988) and KENO-V (ORNL, 1984, Book II, Section F11), are Monte Carlo

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codes for evaluating neutron interactions for highly irregular shapes encountered in criticality safety calculations; the codes are used in this report without modification.

Repository as Steady-State Reactor. The second type of calculations attempted to bound the magnitude of potential energy in the repository by assuming a reactor at steady state for 10,000 yr. Because water is essential for moderating the nuclear reaction (water slows down neutrons so that they have a higher probability of causing a fission of ^{235}U), the energy necessary to boil water was assumed as the maximum output of the reaction. This assumption means that no more than 1 kW of power at steady state could be generated in a natural reactor, which corresponds to about 1 mg/day of ^{235}U or 3.65 kg in 10,000 yr. The energy produced corresponds to about 10^{25} fissions in 10,000 yr, assuming that there are periods within 10,000 yr under which conditions within or near the container can generate a critical condition (see Chapter 10 and Appendix B).

Reactor Dynamics. Although the simple calculations above bound the maximum energy release over 10,000 yr, it would appear unlikely that a natural reactor could produce that energy uninterrupted over such a long time period. Maintaining a critical condition would most likely depend upon maintaining a sufficient amount of water to moderate the reaction (since a "dry" criticality is very unlikely), dissipate heat, and to a lesser extent, remove products from the fission process that absorb neutrons. Changes to any of these processes could stop the reaction until conditions conducive that a new reaction would occur. Evaluating the energy release from this dynamic situation became the goal of the third criticality model.

A complete evaluation of the processes leading to a critical condition should include dynamic changes in the controlling parameters: fuel amount, fuel shape, water, and temperature. Although a fully coupled model monitoring these four aspects was beyond the scope of the 1994 PA, some calculations with a point kinetics code, RNK, developed specifically for the 1994 PA, were manually coupled with the thermal and hydrologic flow codes used for the unsaturated zone in the Complex PA (see Section 1.7.3). This coupling of the nuclear kinetics with the thermal and hydrologic flow code is an important improvement over calculations performed in the past for evaluating critical conditions in the natural environment. These calculations explored how much time was needed after a critical event for optimal conditions to reoccur, i.e., for temperatures to drop and sufficient water to collect again in a zone surrounding a mass of fissile ^{235}U . Preliminary calculations indicated that self shut-down effects are very sensitive to changes in groundwater saturation. Thus, it was not possible to identify any significant energy releases with fully coupled dynamic analysis. To obtain some upper bound results, the critical event was assumed to be between 10^{19} and 10^{21} fissions, which is similar to the release observed in documented criticality accidents. For example, a power period of 4 days and a cycling time period of 71 days was determined assuming 10^{19} fissions in each event, which results in a maximum energy release over 10,000 yr of about 10^{24} fissions, an order of magnitude decrease from the steady-state reactor.

Consequences. The postulated consequences included (a) producing fission products that added to the radionuclide inventory, (b) generating heat that enhanced radionuclide movement, (c) generation of fission gases, and (d) physically damaging the host rock through rapid pressure rises and thus diminishing its ability to contain radionuclides. The latter consequence was considered unlikely because damage would occur only if critical conditions were reached suddenly, releasing energy fast enough to create sufficient steam and pressure to fracture a relatively porous rock. The finding from the study that the possibility of a criticality condition was extremely sensitive to saturation, which in turn was sensitive to temperature because the system was unpressurized, implies that the probability of such an event occurring is low (see Chapter 10 and Appendix B). Thus, in the 1994 PA the consequences of fission production and heat generation were examined and damage to the host rock was neglected. This effect can be examined in future studies.

1.7.3 Corrosion and Source Term Modeling

Most phenomena associated with the waste parcel are included in the gas consumption and source term codes, GASSNF and USATCONC, which are submodels to the flow and transport codes. GASSNF was slightly modified from the version used in the 1993 PA. USATCONC is a completely new source term model that replaces the code used in the 1993 PA, CONCSNF.

Capabilities of Submodels. These submodels, which are described in Chapter 11, include such capabilities as (1) full radioactive decay with any number of radionuclides, (2) defining many different waste packages each with different protective and nonprotective layers and different matrices containing the radionuclides, (3) basing the amount of water for corrosion on calculated saturation in fractures at each time step, (4) defining wet and dry anoxic and oxic corrosion (however only oxic corrosion was used in the 1994 PA), (5) temperature dependence of corrosion rates, (6) diffusion through rubble around the waste containers, and (7) radionuclide sorption on corroded container (iron in 1994 PA). The same submodels are used for the Simple and Complex PAs.

Geochemical Modeling. A potential advantage of the tuff as a host rock is the silica concentration of waters migrating through the strata. Aqueous silica acts as a buffering agent on the system pH, lowering radionuclide solubilities. In addition, uranyl silicate precipitates act as a limiting phase lowering the solubility of uranium by several orders of magnitude. The potential advantage of silica was not incorporated into past performance assessments situated in tuffaceous rock, but the 1994 PA has attempted to do so.

In the 1994 PA, it is assumed that water inside some waste containers would not be saturated with silica since numerous minerals are present that could combine with the silica (thus solubilities used in past performance assessments would apply inside the container). Waters outside the container are assumed to be saturated with silica and thus radionuclides dissolved into the outside waters would have a lower solubility. EQ3/6, a geochemical modeling code used to simulate interactions of groundwaters and solid phases in the natural environment, was used to help evaluate chemical reactions occurring in an open-system, variable-temperature, unsaturated environment (Wolery, 1992a; 1992b).*****

Because of the very complicated nature of geochemical modeling, several solubility experiments conducted with water found in the area (water from the J-13 well) were simulated with EQ3/6 to develop an understanding of the code. (These simulations are described in Appendix E, "Scoping Calculations.") Much experimental data exist evaluating radionuclide solubility in waters with an initial saturation of silica, but at present, no experimental data exist maintaining the silica concentration at saturation levels. EQ3/6 was used to model waters with silica levels maintained close to saturation and to evaluate the solubility of three radionuclides, neptunium (Np), plutonium (Pu), and uranium (U). The resulting range of solubilities over a range of initial pH and reduction and oxidation potentials (Eh) were used to modify the distribution of solubilities from those in TSPA-1993 (Wilson et al., 1994). For instance, the solubility ranges for Np, Pu, and U were assumed to be 10^{-8} to 10^{-2} , 10^{-10} to 10^{-6} , and 10^{-8} to 10^{-2} in the TSPA-1993 yet were found to vary within a range of 3×10^{-7} to 7×10^{-7} , 2×10^{-13} to 1×10^{-12} , and 2.5×10^{-9} to 2.0×10^{-8} , respectively, in the presence of silica (all units in mole/m³ [mM]). In addition, geochemical modeling was performed to evaluate likely forms of uranium that might be precipitated out of solution in silica-saturated water and thus to determine atom ratios for criticality modeling, described in the previous section.

1.7.4 Flow and Transport Modeling

Flow and transport codes are used to model phenomena related to migration of radionuclides away from the container. The gas consumed during corrosion and the amount of radionuclides released from the container are calculated in the corrosion and source term submodel and passed to the flow and transport modeling codes. Because volcanic tuff is potentially highly fractured, the mathematical models that underlie the computational models (i.e., the codes) for both the unsaturated and saturated flow regimes are special cases of a dual-permeability model. Also referred to as a dual continuum, a dual-permeability model consists of a fracture system and a matrix system that are fully coupled in properties such as pressures of each phase, temperatures, and velocities.

In the unsaturated zone, the composite porosity simplification (also called equivalent porosity) of the dual permeability model is used, i.e., the fractures and matrix are assumed to be in local thermodynamic equilibrium. Thus, pressure and temperature in the two media are not calculated separately; instead, a single saturation and permeability function is used that is a function of the properties of the fracture and matrix media (Peters and Klavetter, 1988;

*****The source-term submodel, USATCONC, evaluates radionuclide concentrations inside the container and the unsaturated transport code, NUTS (see Figure 1-9 and Chapter 12) evaluates concentrations outside the container using solubilities of the radionuclides as input. EQ3/6 was not part of the suite of codes used to evaluate the performance of the tuff disposal system; instead, it was used to develop input for NUTS.

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Pruess et al., 1990). Because the unsaturated transport code, NUTS, uses a full dual-permeability formulation, its evaluation of contaminant transport must estimate the fracture and matrix fluid velocities from the composite velocities by using the corresponding capillary pressure curves, as explained in Chapter 12.

Changes to the Complex PA codes from the 1993 PA versions include adding the composite porosity formulation to BRAGFLO_T^{†††††} and completing an unsaturated transport code, NUTS, based on the full dual-permeability formulation. For the Simple PA, most codes are new. TOSPAC (Dudley et al., 1989), the modeling code from Yucca Mountain Project's TSPA-1993 (Wilson et al., 1994), already contained the composite porosity formulation but required coupling with the WIPP modeling system, CAMCON. Also, an abstraction of the results from the 2-D modeling of gas flow was evaluated with GASTP. The linkage of these models is depicted in Chapter 7.

In the transport calculations for the saturated zone, the dual-porosity simplification of the dual-permeability model is used, i.e., the permeability of the matrix is assumed to be zero. Thus, fluid can flow only within the fractures. Without fluid advection in the matrix, diffusion of contaminants occurs only through the pores of the matrix and is orthogonal to the fractures. This special case is implemented in STAFF3D (Huyakorn et al., 1992) for the Complex PA. The one-dimensional single phase transport code, QEDTP, which was used in scoping calculations for the 1993 PA, is run in the Simple PA.

The most recent Sandia evaluation of the potential repository at Yucca Mountain, TSPA-1993, examined a second conceptual model for percolation of water through pores and fractures in the unsaturated zone of the tuff: a weeps model. While the composite-porosity model assumes percolation in both the matrix and the fractures, the weeps model assumes percolation occurs entirely in the large connected fractures of the tuff. Although concurrence has not been reached on the validity of the two models, the composite-porosity model appears to be more readily accepted as a description of percolation in the tuff flow region at Yucca Mountain. The composite-porosity model also promotes a larger release of radionuclides. The weeps model may be better applied to a wetter environment; it can also generate more flow at one location in comparison to the composite-porosity model. This latter point means that the model may promote conditions that are more conducive to a criticality in a waste container. Given the scope of the 1994 PA, only the composite-porosity model was used. However, infiltration at the surface was concentrated at one point in the repository to produce larger percolation, thus potentially promoting conditions conducive to a criticality. Use of the weeps model itself may be of benefit in a future performance assessment.

The 1994 PA assumed that the primary effect of increased infiltration in the composite-porosity model was increased percolation through the repository. A secondary effect, which was not examined due to time constraints, was that the water table might rise. Without a detailed regional model of the area around the proposed repository, a value for the rise itself can only be guessed at. It might be desirable to address this condition in future performance assessments, because complete flooding of the repository contains implications regarding criticality, as shown in the fault tree (Appendix B).

1.7.5 Biosphere Modeling

GENII-S (Leigh et al., 1993), a personal computer version of the software code GENII (Napier et al., 1988a,b,c), was used to evaluate the migration of radionuclides that escape to the accessible environment and eventually reach humans through food or water consumption or related activities. In the 1994 PA, dose calculations were run for the tuff disposal system as well as the salt and granite disposal systems, which were evaluated as part of the 1993 PA. In the 1994 PA, present day conditions and habits of people who reside near the disposal system were assumed to prevail for the next 10,000 yr (the regulatory period for individual doses in 40 CFR 191). This assumption, which eliminates a large source of uncertainty, is based on the philosophy that the contents of a repository would be most hazardous to a society of people with similar technical capabilities and habits. The theory has been advanced that a more primitive society would not be able to contact the waste because they would lack necessary technologies, such

^{†††††}To verify the applicability of the results of the current version of BRAGFLO_T, work was begun on an experimental version of BRAGFLO_T that uses a full dual-permeability formulation. The completion of this task, however, was beyond the scope of this year's work.

as drilling, while a more advanced society would likely not only be aware of the contents but would also have technologies to contend with the hazards currently associated with the waste.

Even with the assumption of present day conditions and habits of people, however, more information is required and uncertainty exists. However, for the 1994 PA, only the uncertainty in parameters associated with the disposal system were included. The parameters associated with the accessible environment were fixed, and the uncertainty and its influence on the individual dose results were not evaluated.

A description of the models and biosphere data is provided in Chapter 14. The results for doses to humans from radionuclides escaping from the disposal systems are presented in Chapter 15.

1.8 Regulatory Assessment

Regulatory assessment consists of evaluating the performance criteria and comparing these results to the regulatory criteria. However, fixed regulations are not currently available (see Section 1.2, Legal Setting). While taking congressional policy into account, the 1994 PA uses two criteria from the 1993 version of 40 CFR 191, containment requirements and individual protection requirements, and two criteria from the unmodified version of 10 CFR 60, waste package and engineered barrier criteria. Of these criteria, the requirements most likely to change substantially are the containment requirements that specify limits on cumulative releases. However, their inclusion here is important for reasons of continuity with previous work.

The Containment Requirements of 40 CFR 191 are probabilistic in nature. Thus, in comparing the performance measures to these regulatory criteria, estimated probabilities of various scenarios (Section 1.6, and Chapters 7 and 8) are combined with estimated measures from the consequence modeling (Section 1.7 and Chapters 9 through 13). The combination produces the probability of the values exceeding those specified by the regulations and is called an exceedance probability curve or a complementary cumulative distribution function (CCDF). Also, because the values of parameters for both the consequence and probability models can be uncertain (which is represented by a distribution of values for each parameter), the performance measure, the CCDF, is also uncertain (and also represented by a distribution). For comparison with the Containment Requirements, the mean of the distribution was used. Because the mean CCDF at the maximum 5-km boundary was quite small, the mean CCDFs at several intermediate points were also evaluated and presented. These CCDFs included the dissolved radionuclide releases from the engineered barrier, releases reaching the water table below the repository, and releases 1, 2.4, and 5 km from the repository in the saturated zone. Gaseous releases of $^{14}\text{CO}_2$ at the engineered barrier and at the surface were also evaluated.

Similarly, the performance measure of maximum annual individual dose can be represented by a distribution of CCDFs. However, the individual protection criteria state simply that the mean of the releases from the disposal system of the scenario without any anthropogenic disturbance must be below 150 μSv . Hence, the performance measure is reduced to a single number for comparison.

The 10 CFR 60 regulation does not specify whether the mean, median, or some other measure of the distribution of the results from the stochastic analysis is to be used for comparison with the criteria for the waste package and engineered barrier. Although the 1994 PA calculated the full distribution of failure times and releases and displayed the mean, median, and 90th quantile of this distribution, the mean was used for comparison. Also, although the calculated release rate is sensitive to the time period over which the rate is calculated, these periods are not specified. To keep the calculations manageable, the 1994 PA calculated the release rate using the large time steps that are selected automatically by the computer code. Because of the required modification to the regulation as a result of the Energy Policy Act of 1992, answers to these questions may be clarified in the future.

For the actual license application of a site, the absolute position of the results compared to the above regulatory criteria is crucial, but this is not the case for this performance assessment. The results are to be used not to determine compliance but instead as a means to gain a measure of insight about the tuff disposal system. The results, therefore, serve as a tool for making rational decisions regarding resource allocations for characterizing spent fuel and high-level waste and for evaluating the current disposal option of minimal waste treatment. Thus, the results of most

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importance are (1) the relative position of the performance measures with respect to the reference waste form, DOE high-level waste in borosilicate glass, and (2) the relative importance of model parameters in determining the value of the performance measure. The latter information is discovered through sensitivity/uncertainty analysis (Section 1.9). The results of the regulatory assessment are discussed further in Chapter 15.

1.9 Sensitivity/Uncertainty Analysis

Sensitivity analysis is used to determine the effect of varying model parameters on the consequences, $C(x, S_j(x))$. Uncertainty analysis involves determining the contribution (importance) of each individual parameter (x_n) to the associated uncertainty of the consequences (distribution of $C(x, S_j(x))$) (Morgan et al., 1990, p. 172) and is primarily used in this report. Both analyses are strongly influenced by the parameter range, but uncertainty analysis also includes the likelihood that the parameter will reach the endpoints of its range. The uncertainty analysis reported herein basically includes creating scatterplots and developing regression models between the parameters and the various results (see, for example, Helton et al., 1992) and using the absolute values of standardized regression coefficients (or the mathematically related partial correlation coefficients) from regression models.

The simplest technique for sensitivity/uncertainty analysis is the scatterplot. A scatterplot is a plot of the results (dependent variable value) vs. model parameters (independent variable value).^{#####} When no relationship exists between the dependent and independent variables, the individual points are incoherently scattered over the plot or spread along a horizontal line. In contrast, the existence of a well defined relationship between the dependent and independent variables is revealed by patterns in the distribution of the individual points.

In stepwise regression analysis, a sequence of regression models is constructed. The first regression model contains the single independent variable with the largest coefficient of determination (r^2) vs. the dependent variable, where the coefficient of determination equals the fraction of the total variability in the dependent variable that can be accounted for by the independent variable. The order in which the independent variables are selected in the stepwise procedure provides an indication of variable importance. Further, the absolute values of the standardized regression coefficients (SRCs) in the regression models also provide an indication of variable importance. Regression on the corresponding ranks of dependent and independent variables was also used to evaluate variable importance, a technique that has proved useful when relationships between dependent and independent variables are highly nonlinear, as is the case with many of the models reported here (Iman and Conover, 1979).

Four important purposes of the sensitivity/uncertainty analysis are (1) to gain understanding and insight about the disposal system, (2) to help verify the correctness of the calculations, (3) to evaluate the influence of various options for spent fuel and high-level waste forms on the results, and (4) to provide input so that decision makers can allocate resources for collecting data about those parameters that most influence the results, based on what is already known about the site or spent fuel and high-level waste. Because uncertainty and sensitivity analyses are inherently conditional on the models, data distributions, and techniques used to generate them, they cannot provide insight about parameters not sampled, conceptual and computational models not used in the analysis in question, or processes that have been oversimplified in the analysis. Hence, qualitative judgment about the modeling system must be used in combination with the results of sensitivity/uncertainty analyses to set priorities for additional data acquisition and model development. The sensitivity/uncertainty analyses are discussed along with other results in Chapter 15.

1.10 Relationships with 1993 PA and Performance Assessments of the Yucca Mountain Project

The 1994 PA can be compared not only to the 1993 PA, but also to previous performance assessments of the Yucca Mountain Project. The similarities and differences in techniques are summarized below.

^{#####}The terms "dependent variable" and "independent variable" refer to the result and the model parameter, respectively. However, the term may be applied differently in some cases to highlight relationships, e.g., the rank of a result may become the dependent variable, or the rank of two or more model parameters mathematically combined may become the independent variable.

Comparison Between 1993 and 1994 PAs. The methodology for the 1994 PA is the same as that used in the 1993 PA which, in turn, is based upon the methodology developed for the performance assessment of the Waste Isolation Pilot Plant (WIPP) Project near Carlsbad, NM. Differences between the performance assessments are shown in Table 1-3. The major differences are that tuff is being modeled as the geologic barrier and only one waste treatment option for spent fuel is being considered. The latter change was based on results of the 1993 PA, which indicated that all treatment options potentially complied with the Containment Requirements of 40 CFR 191 and that improved performance was seen consistently on all waste types only with extensive treatment. In addition, the 1994 PA expanded or changed the focus of the study in five ways: (1) two waste types were added, Shippingport spent fuel and N-Reactor spent fuel from Hanford; (2) horizontal, in-drift disposal was studied in addition to vertical, borehole emplacement; (3) waste parcels were placed close together in horizontal emplacement so that the rock near the containers is heated to above 100°C; (4) waste package and engineered barrier requirements in 10 CFR 60 and dose calculations were considered in addition to 40 CFR 191 regulations; and (5) the possibility of critical conditions occurring in the repository was examined in preliminary calculations.

Comparison Between 1994 PA and TSPA-1993. The 1994 PA draws upon the 1993 Total-System Performance Assessment (TSPA-1993; Wilson et al., 1994) for the Yucca Mountain Project, which was designed to provide feedback to project participants on the significance of design and site-characterization data in regard to regulatory compliance and, thus, resource allocation. The 1994 PA uses the characterization data for the geologic barrier from TSPA-1993 and runs one of its codes. Differences between the performance assessments are shown in Table 1-4. For example, highly enriched uranium spent nuclear fuel is modeled in the 1994 PA and the repository size is smaller (12,060 vs. 70,000 MTHM). Also, processes are differently modeled, e.g., gas flow is coupled with liquid flow in the 1994 Complex PA. A major difference is that an improved source term model is used in the 1994 PA; this model is capable of accounting for the decay of any number of radionuclides rather than using an a priori adjustment of inventories of transported radionuclides as was done for TSPA-1993. Also, the 1994 PA model evaluates the saturation in fractures around the container to determine corrosion rather than using a sampled value from a subjectively estimated distribution based on the percolation rate.

For reference, many other studies of radioactive waste disposal in unsaturated tuff exist with differing degrees of simplification and styles of calculations (see Wilson et al., 1994, p. 3-4). Performance assessments that are nearing completion are studies by Electric Power Research Institute (EPRI), Golder Associates, INTERA, Nuclear Regulatory Commission (NRC), YMP Performance Assessment Departments of Sandia^{*****} supported by Lawrence Livermore National Laboratory for source term modeling, and Pacific Northwest Laboratory (PNL) (see McGuire et al., 1990, 1992; Miller et al., 1992; Intera, 1993; Codell et al., 1992; Barnard et al., 1992; Wilson et al., 1994; and Eslinger et al., 1993). The EPRI, Golder, and INTERA studies use simple models; the Golder and INTERA models are able to simulate all scenarios of the entire disposal system at once. The PNL approach uses detailed multidimensional models of flow and transport but evaluates consequences for only a limited number of model parameters. The NRC and TSPA-1993 are considered intermediate in their degree of simplification.

*****The Performance Assessment Departments for the Yucca Mountain Project and the WIPP Project are both within the Nuclear Waste Management Center of Sandia National Laboratories. The style of their calculations differs as the result of the stage of their respective projects (e.g., Yucca Mountain Project is just starting site characterization, while WIPP's characterization is nearing completion) and the specific requests made by their respective DOE sponsors.

1. Introduction

Table 1-3. Comparison Between 1993 and 1994 INEL Performance Assessments

	1993 PA	1994 PA
Geologic Barrier	Granite and Salt	Tuff
Media	Horizontal pancake strata	Tilted, pancake strata
	No retardation	High retardation except for ^{129}I , ^{99}Tc
Modeling	2 components, no phase changes; single porosity	2 components, phase changes; composite porosity
Engineered Barrier		
Waste Parcel	Evaluate waste treatment options; 5 groupings; 26 waste forms	Evaluate one basic waste form; some modifications, glass and glass-ceramic for calcine; solubility in silica-saturated water evaluated
Waste Forms		
Waste Types	INEL spent fuel (graphite, HEU, LEU) and high-level waste (calcine), and DOE high-level waste (glass)	INEL spent fuel (graphite, HEU, LEU, and Shippingport) and high-level waste (calcine); Hanford spent fuel (N-Reactor); and DOE HLW (glass)
Containers	One container: 1. 9.5-mm thin-shelled stainless steel handling container 2. Optional titanium (salt) or Inconel (granite) overpack	Three containers designed to meet 10 CFR 60 criteria: a. 125-ton MPC for horizontal emplacement 1. 24.5-mm stainless steel handling container 2. Optional 20-mm Incoloy 825 overpack 3. 100-mm carbon steel overpack b. LWT for vertical emplacement 9.5-mm stainless steel handling container Same thicknesses of overpacks as MPC c. 9.5-mm thick stainless steel handling container, over-packed for calcine with same thickness as MPC.
Repository Size	10,000 MTHM (Waste Disposal Group 1)	12,060 MTHM
Orientation	Vertical	Vertical and Horizontal
Layout	WIPP-like (rooms grouped as panels)	YMP-like (uses tunnel-boring machine); Horizontal - 4.3-m dia. drifts Vertical - 7.65-m-dia. drifts
Regulatory Criteria (based on regulations that are currently being revised)		
Total System	40 CFR 191; 10,000-yr Containment Requirements No dose calculation except for demonstration	40 CFR 191 10,000-yr Containment Requirements 10,000-yr Individual Protection Requirements; dose calculated from several pathways for salt, granite, tuff disposal systems

Table 1-3. Comparison Between 1993 and 1994 INEL Performance Assessments (Continued)

(Regulatory Criteria, continued) Components	1993 PA	1994 PA
	None	10 CFR 60 waste package and engi- neered barrier requirements
Features, Events, Processes Scenarios		
Non-criticality	10,000-yr regulatory period Features: brine reservoir (salt); frac- tures (granite)	10,000-yr regulatory period Tuff (unsaturated), climate change process Features: fractures
Criticality	None in container since limited fissile mass or in far-field	Assumed in or very near container; Far-field - none

Table 1-4. Comparison Between TSPA-1993 and INEL Complex and Simple 1994 PAs

TSPA-1993 (Wilson et al., 1994)	INEL 1994 PA (Complex and Simple PAs)
Engineered Barrier	
Waste Parcel	
Waste Form	
1. Source term (YMIM) <ul style="list-style-type: none"> - Rough approximation of decay (no ingrowth so inventory must be adjusted for radionuclides transported) - One waste parcel - Saturation near container function of percolation rate, but not used by YMIM - Wet and dry oxid corrosion - Temperature dependence of corrosion rates - No diffusion through failed layers - No radionuclide sorption on corroded iron (could be modeled in fluid flow code) 	1. Source term (USATCONC) <ul style="list-style-type: none"> - Full radionuclide decay with any number of radionuclides (currently 32) not just those transported - Many individual or mixed waste packages with different protective and nonprotective layers and matrices - Inventory may be in several locations - Water for corrosion based on calculated saturation in fractures from composite porosity model - Wet and dry anoxic and oxid corrosion - Temperature, O₂, water saturation, and time dependence of corrosion rates - 1D diffusion modeled through rubble contacting container - Radionuclide sorption on corroded iron - Separate solubility inside and outside container - Fraction of container layers or fuel cladding may have failed - Rate or solubility control for matrix alteration - Special output for release rates, removal of fissionable material or neutron absorbers, breach times
2. Waste Intermingled <ul style="list-style-type: none"> - Spent fuel (commercial low enriched): 63,000 MTHM - DOE high-level waste (glass): 7000 MTHM 	2. Waste Intermingled (Complex PA) <ul style="list-style-type: none"> - INEL spent fuel (graphite, HEU, LEU, and Shippingport); 370 MTHM - INEL high-level waste (calcine in glass ceramic); 320 MTHM - Hanford spent fuel (N-Reactor); 2100 MTHM - DOE high-level waste (borosilicate glass); 9270 MTHM Waste studied separately (Simple PA)
Container	
3. Horizontal Emplacement <ul style="list-style-type: none"> - MPC (1.53 m dia by 4.90 m long) of 9.5-mm Incoloy 825 - 100-mm mild carbon steel overpack 	3. Horizontal Emplacement <ul style="list-style-type: none"> - 125-ton MPC (1.53 m dia by 4.90 m long): 25.4-mm 304L stainless - 100-mm carbon steel overpack - Optional 20-mm Incoloy 825 overpack
4. Vertical Emplacement <ul style="list-style-type: none"> - 9.5-mm thick canister (0.71 m dia by 4.76 m long) 	4. Vertical Emplacement <ul style="list-style-type: none"> - DOE glass in 9.5-mm thick stainless steel canister (0.61 m dia by 3 m long) - Other waste in 25-ton LWT container (0.47 m square by 4.6 m long) with same materials and thicknesses as MPC, except handling container is 9.5 mm thick

Table 1-4. Comparison Between TSPA-1993 and INEL Complex and Simple 1994 PAs (Continued)

TSPA-1993 (Wilson et al., 1994)	INEL 1994 PA (Complex and Simple PAs)
Repository	
5. Size - 70,000 MTHM 6. Orientation - parallel with tilted stratigraphy 7. Areal power density - 14.1 W/m ² (57 kW/acre) - 28.2 W/m ² (114 kW/acre) 8. Extraction ratio ~30%	5. Size - 12,060 MTHM 6. Orientation - parallel with tilted stratigraphy 7. Areal power density - Vertical - 14.1 W/m ² (57 kW/acre) - Horizontal - 23.5 W/m ² (tightly packed MPCs) 8. Extraction ratio ~42%
Geologic Barrier	
Unsaturated Zone	
9. Stratigraphy calculated by geostatistics, but only one realization used; repository divided into eight 1-D simulations 10. Two fluid flow conceptual models: (a) composite porosity and (b) weeps 11. Gas transport - Coupled with heat effects in 2-D model but decoupled from 1-D liquid flow - ¹⁴ C exchange with bicarbonate acid included as effective Kd $^{14}\text{CO}_2 \rightleftharpoons \text{H}_2\text{CO}_3$ 12. Radionuclides transported (8): ¹⁴ C, ¹²⁹ I, ²³⁷ Np, ²³¹ Pa, ²³⁹ Pu, ⁷⁹ Se, ⁹⁹ Tc, ²³⁴ U (¹²⁹ I, ⁹⁹ Tc essentially nonsorbing, nondecaying tracers) in first 10,000 yr	9. Horizontal "pancake" stratigraphy in 2-D Complex PA; one 1-D simulation for repository in Simple PA 10. One flow conceptual model - composite porosity 11. Gas transport - ¹⁴ C exchange with bicarbonate acid included as effective Kd $^{14}\text{CO}_2 \rightleftharpoons \text{H}_2\text{CO}_3$ - Complex PA - directly coupled with heat effects in 2-phase 2-D model - Simple PA - abstraction of TSPA-1993 work 12. Radionuclides transported (12): ¹⁴ C, ¹²⁹ I, ²³⁷ Np, ²³¹ Pa, ²³⁹ Pu, ⁷⁹ Se, ⁹⁹ Tc, ²³³ U, ²³⁴ U, ²³⁵ U, ²³⁶ U, ²³⁸ U
Saturated Zone	
13. Stratigraphy (STAFF3D) - 3D pancake with layers cut off at location of water table to make confined tilted units - single porous medium - no retardation 14. Modeling - only local model - 2 conceptual models a) diversionary b) nondiversionary - steady-state flow field - release point of radionuclides at water at projected center of repository - results abstracted to one-dimensional flow	13. Stratigraphy (STAFF3D) - 3-D pancake with water table - dual porosity - retardation 14. Modeling - only local model - one conceptual model (similar to diversionary) - water table rise included but evaluated separately from unsaturated model (for dose calculations) - steady-state flow and transient fields - release region of radionuclides at water table based on plume in unsaturated zone - TSPA-1993 results abstracted for Simple PA

1. Introduction

Table 1-4. Comparison Between TSPA-1993 and INEL Complex and Simple 1994 PAs (Continued)

TSPA-1993 (Wilson et al., 1994)	INEL 1994 PA (Complex and Simple PAs)
Agents Acting on Disposal System	
15. Climate - wet-dry cycle (step function)	15. Climate - wet-dry cycle
<ul style="list-style-type: none"> - 100,000-yr period - times of wet-dry change sampled - base, peak, and rate sampled from uniform distribution - water table rise sampled 	<ul style="list-style-type: none"> - Complex PA (sinusoidal function) - period sampled (mean of 100,000 yr) - base peak and rate sampled - high infiltration area included at surface
16. Drilling	16. Drilling
<ul style="list-style-type: none"> - extraction sampled (range: zero to entire container) - includes near miss contaminated rock - does not enhance ground water release - individual doses not calculated 	<ul style="list-style-type: none"> - extraction of entire contents of container if hit - excludes near miss contaminated rock - does not enhance groundwater release - individual doses calculated from well located below disposal area and 1000 m downgradient

2. Regulatory Criteria for Radioactive-Waste Repositories

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This chapter discusses the following topics:*

- The Nuclear Waste Policy Act of 1982
- The Energy Policy Act of 1992
- International criteria for radioactive waste disposal
- Environmental Protection Agency's 40 CFR 191
- Nuclear Regulatory Commission's 10 CFR 60
- Hazardous waste disposal standards

If you are familiar with the Environmental Protection Agency (EPA) and Nuclear Regulatory Commission (NRC) regulations, you may want to skip this chapter as it discusses the history of these regulations, as well as their meaning.

Federal regulations governing radioactive-waste disposal are the direct result of United States policy decisions beginning in the 1950s. However, only since the late 1970s have international organizations produced guidelines for the world community that helped in creating radiological standards. The United States was one of the first countries to promulgate radioactive-waste disposal standards when the EPA published 40 CFR 191 in 1985.

Potential changes and additions to the radioactive-waste regulations make it difficult to determine what criteria might be used to regulate future, as yet unspecified repositories. All or parts of these current and proposed requirements could form the basis for regulating additional repositories. Analysts providing performance assessments of generic repositories need to remain aware of requirements and criteria that might apply to future repositories.

The 1993 performance assessment for the INEL Project relied heavily on requirements of 40 CFR 191 to guide its methodology. The value of that performance assessment was in its very broad system analyses of the nuclear waste disposal issue (similar to work performed by the European community [BRWM, 1992, p. 58-62]). For the 1994 iteration, considerable reliance is again placed on requirements in 40 CFR 191. However, the more detailed components requirements of 10 CFR 60 are also considered.

Currently, neither 40 CFR 191, nor 10 CFR 60 applies to Yucca Mountain because the Energy Policy Act of 1992 states that new public health and safety standards protecting the public from radioactive waste will be promulgated for the Yucca Mountain site. These standards will be the only ones applicable to Yucca Mountain. We discuss 40 CFR 191 and 10 CFR 60 in this chapter because they are the only regulations that currently exist that we can use as a baseline. For more information on the *Energy Policy Act of 1992*, see Section 2.1.2. A copy of the act appears in Appendix C. While the legal policy of this act is clear, the regulatory criteria are unknown.

2.1 Nuclear Waste Policy in the United States

Radioactive-waste repositories in the United States must comply with requirements of applicable federal and state regulations. A primary regulation for radioactive-waste disposal is the EPA's *40 CFR 191: Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes* (EPA, 1985a; 1993). The regulation specifies radioactive-waste disposal based on a total system approach. Additional requirements and regulations pertaining to both radioactive- and hazardous-waste disposal must also be considered. The Nuclear Regulatory Commission's (NRC) requirements in 10 CFR 60 call for an evaluation of the isolation capability of a geologic repository in accordance with 40 CFR 191, but also include specifications that regulate engineered- and geologic-barrier subsystems. The *Resource, Conservation, and Recovery Act of 1976* (RCRA) and asso-

* 10 CFR 960 *General Guidelines for the Recommendation of Sites for Nuclear Waste Repositories* is not considered here because this effort is concerned with comparing treatment options for a generic site rather than selecting an actual site.

2. Regulatory Criteria for Radioactive-Waste Repositories

ciated regulations provide for management of waste contaminated with hazardous chemicals. The *Nuclear Waste Policy Act of 1982* and the *Energy Policy Act of 1992* are discussed in the Sections 2.1.1 and 2.1.2, respectively.

2.1.1 The Nuclear Waste Policy Act of 1982

The *Nuclear Waste Policy Act of 1982* (NWPA, 1983) and subsequent amendments of 1987 (NWPAA, 1987) provide a national policy for interim storage, monitored retrievable storage, and eventual disposal of radioactive waste. Thus, while not establishing any performance metrics, the act does specify the approach to nuclear waste disposal to be followed in the United States based on the decision that the current generation has an obligation to bear the political and financial costs of developing a permanent disposal option.[†] In general, the *Nuclear Waste Policy Act* establishes the following four provisions: (1) a detailed schedule for all major decisions related to developing disposal options for spent nuclear fuel and high-level waste; (2) extensive procedures for involving states and the public in all major decisions, while directing the EPA to issue standards and the NRC to issue regulations to enforce those standards; (3) a Nuclear Waste Fund, funded by a tax on electricity from nuclear reactors for development of one repository (two prior to the 1987 amendments) to accept nuclear waste from reactors; and (4) a separate office within the DOE, the Office of Civilian Radioactive Waste Management, to implement the requirements of the *Nuclear Waste Policy Act*.

Two important policy requirements from this act are pertinent to disposal of DOE defense and experimental waste. First, the *Nuclear Waste Policy Act* clearly states that a repository for waste generated by federal defense activities will comply with all requirements of the NRC (i.e., 10 CFR 60) (NWPA, 1983, Section 8). Defense transuranic waste was exempted in 1979 by legislation pertaining to the Waste Isolation Pilot Plant (Public Law 96-164). Second, it assumes that defense waste will be disposed of with commercial waste unless the President of the United States recommends to Congress that defense wastes be disposed of separately. In 1985, the DOE recommended to the President that such waste be disposed of in the same repository as commercial spent nuclear fuel (U.S. DOE, 1985a). President Reagan subsequently made that recommendation.

2.1.2 The Energy Policy Act of 1992

The *Energy Policy Act of 1992* (Energy Policy Act, 1992) provides a plan to establish safety standards that are to apply specifically to the Yucca Mountain site, a proposed repository for the disposal of high-level waste in an unsaturated tuff formation. The standards, aimed at protecting the public from the danger of exposure to radioactive material stored in Yucca Mountain, are to prescribe the maximum annual effective dose equivalent to individuals from release of radioactivity from the repository to the accessible environment. These standards are to be the only ones applicable to Yucca Mountain. In mandating the development and application of new regulations, Congress has set aside 40 CFR 191 in the case of Yucca Mountain.

The act mandates that the National Academy of Sciences (NAS) perform a study to determine whether individual dose is a satisfactory safety criterion, whether a waste site can be maintained adequately to prevent breaching the repository's engineered and geologic barriers, and whether it is possible to predict the likelihood of human intrusion over a period of 10,000 years. The results of this study are expected in April 1995.

Once the NAS has developed their recommendations, the EPA must promulgate standards consistent with these recommendations. In addition, the NRC must modify 10 CFR 60 to be consistent with these new EPA standards and the supporting NAS recommendations, including an assumption that post-closure oversight at the repository will prevent unreasonable risk of breaching the repository. These new regulations are to be the only such standards applicable to the Yucca Mountain site.

[†] The word "option" is emphasized because, although the initial impulse of all impacted by the NWPA was to simultaneously develop an option and fully implement it, current thinking is to develop an option and demonstrate it with a licensed facility, but not necessarily fully implement to give future generations a real choice; there are few reasons to fully implement immediately because the waste can remain safely at reactor sites for approximately 100 years; immediate implementation could foreclose other options such as recycling that future generations may wish to exercise (Isaacs et al., 1993).

1 Congress has taken several steps in recent years that would question existing generic radioactive waste standards.
 2 Currently, in the United States, only two mined geologic repositories for containerized radioactive waste are being
 3 considered—the Waste Isolation Pilot Plant (WIPP) in New Mexico for transuranic waste in bedded salt and the
 4 Yucca Mountain site in Nevada for high-level waste. For both of these proposed repositories, Congress has man-
 5 dated that the EPA will promulgate new regulations (a specific high-level waste standard currently applicable only to
 6 Yucca Mountain, and WIPP-specific regulations to certify compliance with the generic regulations).
 7

8
 9 The EPA's 40 CFR 191 was first promulgated in 1985. Subpart B of the regulation (long-term performance
 10 requirements) was remanded to the EPA in 1987 for further consideration. The EPA repromulgated the revised regu-
 11 lation in late 1993. The EPA is required by the *Waste Isolation Pilot Plant Land Withdrawal Act* to promulgate crite-
 12 ria for implementing 40 CFR 191 for the Waste Isolation Pilot Plant (to be found at 40 CFR 194).
 13

14
 15 An important result of the Energy Policy Act, 1992 is the usage of a maximum annual effective dose equivalent
 16 as a safety standard instead of release limits at the disposal system boundary (as is the current strategy in 40 CFR
 17 191). See Chapter 14 for more information on effective dose equivalents.
 18

21 2.1.3 Environmental Impacts

22
 23 The *National Environmental Policy Act* (NEPA) (NEPA, 1970, as amended) is enforced by regulations that are
 24 not specific regulatory guidelines but contain a mandate for evaluating the environmental consequences of all signifi-
 25 cant aspects of a federal project (EPA, 1978). The DOE has prepared environmental impact statements (EISs) and
 26 environmental assessments that have addressed the predicted experimental, operational, and long-term behavior of
 27 potential repositories (U.S. DOE, 1979; 1980; 1986a,b; 1990). However, the NEPA's impact on the waste-treatment
 28 options themselves will be only indirect because its focus is primarily on the requirements for the siting of processing
 29 plants and deep geologic repositories. Although not explicitly required for an EIS or environmental assessment, eval-
 30 uations of individual doses to the public may be required by the implementing agency to support any decisions of
 31 minimal and acceptable environmental consequences.
 32
 33

34 2.1.4 Regulations, Standards, and DOE Orders on Criticality Safety

35
 36 With regard to disposal of spent nuclear fuel owned by the U.S. Department of Energy, the current view is to dis-
 37 pose of it in a geologic repository without removing or diluting the fissile radionuclides, even though significant
 38 quantities exist in some of the fuels. Hence, disposal of spent nuclear fuel in a repository requires that the possibility
 39 of conditions conducive to criticality be considered. At present, regulations lack statements that address criticality
 40 issues post-closure. In fact, there are no DOE orders addressing these issues. Examples of the types of statements
 41 that would generally address criticality issues include (1) the length of the regulatory period (10,000 yr or longer), (2)
 42 the accepted probability of a critical event, (3) whether assurance requirements should dictate use of certain compo-
 43 nents such as placement of neutron absorbers in the containers, (4) the level of quality assurance necessary regarding
 44 requirements, and (5) the generally accepted style of the calculations for showing compliance.
 45
 46

47
 48 For example, the NRC regulation (10 CFR 60) specifically states that prior to closure:
 49

50
 51 “All systems for processing, transporting, handling, storage, retrieval, emplacement, and isolation of radioac-
 52 tive waste shall be designed to ensure that a nuclear criticality is not possible unless at least two, independent,
 53 and concurrent or sequential changes have occurred in the conditions essential to nuclear criticality safety.
 54 Each system shall be designed for criticality safety under normal and accident conditions. The calculated
 55 effective multiplication factor (k_{eff}) must be sufficiently below unity to show at least a 5% margin, after
 56 allowance for the bias in the method of calculation and the uncertainty in the experiments used to validate the
 57 method of calculation” [§60.131(b)(7)].
 58
 59

60
 61 However, 10 CFR 60 is silent concerning post-closure criticality issues. Furthermore, standards of the American
 62 Nuclear Society/American National Standards Institute (ANS/ANSI), from which the DOE Orders and 10 CFR 60
 63

2. Regulatory Criteria for Radioactive-Waste Repositories

draw their requirements, are explicit about criticality safety requirements, except in a repository after closure. The EPA standard, 40 CFR 191, examines the repository system as a whole and as such implicitly includes this type of issue, but no known precedent-setting calculations existed for use as guidance when the standard was promulgated.

2.1.5 Other Statutes and Regulations

Numerous statutes and regulations that are not specifically discussed can have a tertiary effect on the performance criteria of a geologic repository. These regulations address a wide range of concerns, from packaging and transportation of hazardous and radioactive materials (e.g., 10 CFR Part 71 and 49 CFR Parts 106-179) to protection of the environment through regulations pertaining to clean air (e.g., 40 CFR Part 61), clean water (e.g., 40 CFR Part 141, 40 CFR Part 144, and 40 CFR Part 122), and control of toxic substances (e.g., Toxic Substances Control Act).

2.2 International Criteria for Radioactive-Waste Disposal

This section examines international criteria for radioactive waste disposal. We discuss this topic here because the international community uses individual dose as a safety measure and Congressional guidance has suggested that maximum individual dose should be used as a safety measure in the United State

Radiation protection principles published by international organizations, especially those of the International Commission on Radiological Protection (ICRP), have provided the basis for regulations in countries considering methods for disposal of radioactive waste (Table 2-1). In 1984, the Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development published an expert group report that introduced the concept of a basic individual risk criterion for radioactive-waste disposal (NEA, 1984). The report recommended that protection of the individual should be expressed in terms of risk, where risk was defined as the product of the probability of exposure and the probability that doses received would give rise to deleterious health effects. Individual risk limits were to correspond to the risk associated with the current dose recommendations of the ICRP (NEA, 1984).

The ICRP's recommendations in Report 46 (ICRP, 1985) complemented the 1984 NEA report. In addition, a risk-based criterion was established that accounted for the probability of the dose being received as well as the probability of serious health effects from the dose. The International Atomic Energy Agency (IAEA) subsequently published safety principles and technical criteria for underground disposal sites that use doses as the performance measure (IAEA, 1989). The most recent ICRP principles, published in Report 60 (ICRP, 1990) reiterate these recommendations.

An international consensus now exists on the general radiological protection principles for disposal of radioactive waste. These principles are summarized as the following (NEA, 1991):

Individual risk for members of the public should be limited to a level corresponding to the risk associated with the current ICRP individual dose limit (1 mSv per year). This level corresponds to a risk on the order of 1 in 100,000 of experiencing fatal cancer, when the probability of the events giving rise to exposure and potential health consequences of exposure are considered. For single repositories, a risk target of 1 in 1,000,000 has been adopted by some national authorities.

The ALARA principle (i.e., to keep doses as low as reasonably achievable) should be taken into account as much as possible in overall optimization of the disposal system:

"the magnitude of individual doses, the number of people exposed, and the likelihood of incurring exposures where these are not certain to be received should all be kept as low as reasonably achievable, economic and social factors being taken into account"

Table 2-1. Regulatory Waste-Disposal Objectives/Criteria at the International Level and in Individual Countries (adapted from NEA, 1991)

Organization/ Country	Main Objective/Criteria	Other Main Features	Comments
NEA (NEA, 1984)	For high level waste (HLW), maximum individual risk 10^{-5} /yr (all sources)	Individual risk/dose best criterion to judge long-term acceptability	No consensus on ALARA* optimization
ICRP Publication 46 (ICRP, 1985)	For HLW, for individuals (all sources): 1 mSv/yr (normal evolution scenarios); 10^{-5} /yr (probabilistic scenarios)	Both probability and doses should be taken into account in ALARA	ALARA useful, notably to compare alternatives, but may not be the most important siting factor
IAEA Safety Series 99 (IAEA, 1989)	ICRP Publication 46 (ICRP, 1985)		Also includes qualitative technical criteria on disposal system features and role of safety analysis and quality assurance
ICRP Publication 60 (ICRP, 1990)	Limit for public exposure for individuals should be expressed as an effective dose of 1 mSv/yr	Also advocates justification for any practice involving exposure to radiation, and optimization of protection	
CANADA (AECB, 1987)	For HLW, maximum individual risk objective 10^{-6} /yr	Period of time for demonstrating compliance: 10^4 yr	Additional qualitative, non-prescriptive requirements and guidelines in regulatory documents
FINLAND (Finnish Centre for Radiation and Nuclear Safety, 1991)	For low and medium level waste, maximum individual dose < 0.1 mSv/yr, with maximum individual dose < 5 mSv/yr from accident conditions caused by possible natural events or human actions	Analysis of emissions beyond 1 million years generally not meaningful	For spent fuel or HLW, proposed criterion for maximum individual dose < 0.1 mSv/yr
FRANCE (Basic Safety Rule of 1992)	For both low level waste and HLW, in normal evolution scenario, maximum individual dose < 0.25 mSv/yr		Technical criteria for siting established in 1987
GERMANY (Section 45, para. 1 of Radiation Protection Ordinance, 1989)	For HLW, maximum individual dose < 0.3 mSv/yr for all reasonable scenarios	Calculation of individual doses limited to 10^4 yr but isolation potential beyond 10^4 yr may be assessed	Additional qualitative technical criteria in guidelines and regulatory documents
THE NETHERLANDS	Not yet developed		Recent assessments used dose criteria from other countries, with risk criteria for scenarios with a high dose

* ALARA – as low as reasonably achievable.

2. Regulatory Criteria for Radioactive-Waste Repositories

Table 2-1. Regulatory Waste-Disposal Objectives/Criteria at the International Level and in Individual Countries (adapted from NEA, 1991) (Continued)

Organization/ Country	Main Objective/Criteria	Other Main Features	Comments
NORDIC COUNTRIES (Basic Criteria Document of 1993)	For HLW, maximum individual dose < 0.1 mSv/yr (normal scenarios); maximum individual risk < 10^{-6} /yr (disruptive events)	Additional criterion on "total activity inflow" limiting releases to biosphere, based on inflow of natural alpha radionuclides	Under revision following broad consultation
SWITZERLAND (Regulatory Document R-21, 1980)	For HLW, maximum individual dose < 0.1 mSv/yr at any time for reasonably probable scenarios	Repository must be designed in such a way that it can at any time be sealed within a few years without the need for institutional control	Revision of Regulatory Document R-21 is underway
UNITED KINGDOM (Radioactive Substances Act of 1993)	< 10^{-6} /yr target for individual risk from a single facility (equivalent to that associated with a dose of 0.1 mSv/yr)	No time frame for quantitative assessments specified	ALARA to be used to the extent practical and reasonable
UNITED STATES (EPA 40 CFR Part 191, 1993)	For HLW, spent fuel, and transuranic waste, limits on projected radionuclide releases to the accessible environment for 10^4 yr, based on objective to limit serious health effects to less than 10 in the first 10^4 yr after disposal for each 1000 metric tons of spent fuel or HLW disposed of	Individual dose (over 10,000 yr) < 0.25 mSv/yr Other requirements on drinking water contamination	1985 EPA standards were remanded in 1987 and revised in 1993 for application to the Waste Isolation Pilot Plant; U.S. Congress mandated a new regulation to apply to the Yucca Mountain Project in Nevada for HLW and spent fuel
(NRC 10 CFR Part 60, 1983)	For HLW, minimum levels of performance specified for: waste package ("substantially complete" containment for 300-1000 yr); engineered barrier system (releases < 10^{-5} yr ⁻¹ of the inventory at 1000 yr after repository closure); pre-waste-emplacement groundwater travel time between "disturbed zone" and "accessible environment" > 10^4 yr	Siting criteria for avoidance of foreseeable adverse human activity; separate consideration of anticipated processes and events (naturally occurring) and unanticipated processes and events (naturally occurring or human induced)	NRC subsystem requirements intended to help achieve compliance with EPA standards; U.S. Congress recently mandated consideration of revisions to the regulation specifically for the proposed Yucca Mountain site in Nevada

The Commission also recommends that the exposure of individuals that results from the combination of all the relevant practices should be:

“subject to dose limits, or to some control of risk in the case of radiation risks that are judged to be unacceptable from these practices in any normal circumstances.”

The approaches to application of the general radiation protection principles are largely similar in most countries. Their translation into quantitative safety criteria for radioactive-waste disposal, however, may differ somewhat among the countries (see Appendix D for a discussion of radioactive-waste disposal programs in other countries). Such differences concern the following issues (NEA, 1991):

- the explicit use of limits expressed in terms of dose or in terms of risk
- the use of individual and/or collective dose/risk limits
- the level of detail of the criteria (e.g., use of subsystem criteria and special criteria for certain scenarios)
- the period for which compliance has to be shown

All existing regulations use either dose or risk (or both) as a fundamental measure of performance (NEA, 1991). The NEA, ICRP, and IAEA principles (NEA, 1984; ICRP, 1985; IAEA, 1989) express the idea that assessments of radioactive-waste disposal should consider not only the most likely scenario and related expected releases, but also a set of scenarios that are uncertain or even unlikely to happen. The ICRP recommendations use the risk concept to propose a constraint on the annual individual risk of severe health effects at a level of about 10^{-5} (consistent with the risk implied by the annual dose limit recommended for individual members of the public). Several national regulations (e.g., the United Kingdom and Canada) explicitly follow this recommendation but set the risk limit at 10^{-6} for radioactive-waste disposal practices based on the belief that waste disposal is only one of several potential sources for exposure. These risk levels are shown in Figure 2-1. Some countries have also chosen to use dose limits for high-

Probability of
Human Health
Effects/Yr

International Commission on Radiologic Protection (ICRP) Nuclear Energy Agency (NEA), and International Atomic Energy Agency (IAEA) recommended limit

Design target
High-level and low-level repository probabilistic safety assessments by Canada, Finland, Germany, Sweden, Norway, and the United Kingdom

TRI-6342-3843-1

Figure 2-1. Acceptable risks permitted internationally assuming 5×10^{-4} health effects per rem.

2. Regulatory Criteria for Radioactive-Waste Repositories

probability scenarios and to consider low-probability, disruptive scenarios separately. Thus, several countries (e.g., Switzerland and Germany) have regulations using dose limits and make no explicit use of risk criteria. However, using dose limits does not necessarily mean that these countries do not recognize the need to consider the risks associated with probabilistic events and the need to try to estimate them when appropriate (NEA, 1991). Doses from various sources are shown in Figure 2-2.

Only limited use has been made of collective dose or risk in safety criteria and assessments (NEA, 1991). Use of collective dose/risk requires assumptions not only about future critical groups of humans and their habits, but also about the whole society (e.g., number of people and their living conditions and habits). Collective dose calculations are associated with large uncertainties, and differences among disposal options could be masked by the uncertainty ranges affecting such calculations. Most countries generally regard individual dose or risk limits as more appropriate for determining long-term acceptability of high-level waste disposal practices, with collective dose or risk limits used mainly as a comparison tool for the discussion of repository design alternatives (NEA, 1991).

Few countries use specific quantitative criteria for regulating the performance of subsystems within a disposal system. Any derived criteria usually are expressed in qualitative terms so that the regulator can provide guidance without specifying required subsystem performance (NEA, 1991). The philosophy for using only qualitative criteria for subsystems is that detailed quantitative regulations for subsystems might be premature or even counterproductive to a flexible and gradual process of developing the repository system and establishing the optimal balance between different barrier functions (NEA, 1991). As discussed in Section 2.4, in the United States the NRC has included specific quantitative criteria for subsystem performance that serve as default specifications for achieving a required level of performance. However, the NRC regulations explicitly provide for approval of alternative subsystem criteria, if appropriate (10 CFR 60.113[b]).

TRI-6342-3414-3

Figure 2-2. Dose comparisons from various sources.

All countries examine potential radiological impacts over long time frames (NEA, 1991). Formal requirements for quantitative assessment up to at least 10,000 years are included in some regulations (e.g., Canada, Germany, and the United States). Other countries do not use such "cut-off" times and consider quantitative assessments for one million years (e.g., Finland) or even longer. However, most of the regulations also indicate the recognition of the following two factors that influence the type of approach required to demonstrate and judge compliance with basic protection principles: (1) uncertainties associated with assessment results increase with time; and (2) radioactivity of the waste decreases with time. These two trends suggest that detailed quantitative assessments become less meaningful over increasingly longer time periods. Thus, some regulators have indicated that detailed quantitative assessments, including dose calculations, are justified for shorter periods, while a less detailed, more qualitative approach should be used for times far into the future (NEA, 1991).

2.3 Overview of EPA's Regulation, 40 CFR 191

Although 40 CFR 191 is not applicable to Yucca Mountain as a result of the Energy Policy Act, 1992, we describe it here because we have no other criteria on which to base the performance assessment. We use the criteria set forth in 40 CFR 191 in the performance assessment; therefore, it is important to understand this standard.

2.3.1 Organization of 40 CFR 191

The EPA regulation for radioactive-waste disposal (40 CFR 191) is divided into three subparts. Subpart A limits annual radiation doses to the public during the operational period of the facility.

Subpart B of 40 CFR 191 provides long-term performance measures for the entire disposal system rather than for individual components. Subpart B establishes Assurance Requirements (design and control philosophy that includes a multiple-barrier concept), post-closure Individual Protection Requirements (maximum annual radiation dose to the public from an undisturbed repository for 10,000 years), and post-closure Containment Requirements (probabilistic release limits for 10,000 years).

Subpart B of 40 CFR 191 does not apply to any repository characterized under the Nuclear Waste Policy Act, 1982, as amended. This indicates that if a second repository is licensed for commercial waste under the auspices of the Nuclear Waste Policy Act of 1982, it could be regulated under the new EPA Yucca Mountain regulation, or possibly its own site-specific regulation.

Subpart C provides Environmental Standards for Groundwater Protection (maximum radionuclide concentrations in underground sources of drinking water for 10,000 years). The text of 40 CFR 191 is in Appendix C of this report.

The radioactive-waste disposal standards originally promulgated by the EPA in 1985—*40 CFR Part 191: Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes* and repromulgated in 1993 after legal proceedings (EPA, 1985a; 1993)—are divided into three subparts (Figure 2-3). Subpart A applies to a disposal facility prior to decommissioning. Subpart B applies after decommissioning and contains the following quantitative and qualitative requirements for long-term performance of a repository:

- The Containment Requirements (§191.13) set limits on the probability that cumulative releases of radionuclides beyond the "controlled area" (defined in the regulation as a surface location that encompasses no more than 100 km² and extends horizontally no more than a 5-km radius from the outer boundary of a radioactive-waste disposal system, plus the underlying subsurface [§191.12] [see Figure 2-4]) for 10,000 years after disposal) will be exceeded. The regulation specifies a reasonable expectation that the limits will be met.
- The Assurance Requirements (§191.14) are qualitative requirements that specify actions and procedures to increase confidence "because of the inherent uncertainties in selecting and designing disposal systems that

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Figure 2-3. The EPA's 40 CFR 191—Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes (EPA, 1993).

must be very effective for more than 10,000 years" (EPA, 1985a, p. 38069). These requirements apply only to disposal systems not regulated by the NRC, because comparable provisions exist in NRC regulations (see Section 2.4).

Each Assurance Requirement applies to some aspect of uncertainty about long-term containment. They are as follows:

- Limiting reliance on active institutional controls to 100 years precludes relying on future generations to maintain surveillance.
- Carefully planned monitoring will increase the likelihood of unexpectedly poor system performance being detected.
- Using passive institutional controls such as markers and records will reduce the chances of inadvertent or systematic intrusion.
- Including multiple barriers, both engineered and natural, will reduce the risk of leakage should one type of barrier fail.
- Considering the disposal site's future resource potential and demonstrating that the favorable characteristics of the disposal site compensate for the likelihood of disturbance will add to the confidence that the chosen site is appropriate.
- Selecting a disposal system that permits possible future recovery of most of the wastes for a reasonable period of time after disposal will allow future generations the option of relocating the wastes should new developments warrant such recovery.

Figure 2-4. Artist's concept of a mined geologic disposal system portraying terminology used in 40 CFR 191, Subpart B and this report (modified from Bertram-Howery and Hunter, Eds., 1989, Figure II-1).

2. Regulatory Criteria for Radioactive-Waste Repositories

We are not using assurance requirements as criteria in the performance assessment. Therefore, we will not discuss them further.

- The Individual Protection Requirements (§191.15) set limits on radiation doses to members of the public received through all potential pathways from the disposal system to the accessible environment (the environment beyond the controlled area [§191.12]) for 10,000 years of undisturbed performance after disposal. The regulation specifies a reasonable expectation that the limits will be met.

Subpart C, Environmental Standards for Groundwater Protection, set limits on concentrations of radioactive contaminants in underground sources of drinking water in the accessible environment during 10,000 years of undisturbed performance after disposal:

“Disposal systems...shall be designed to provide a reasonable expectation that 10,000 years of undisturbed performance after disposal shall not cause the levels of radioactivity in any underground source of drinking water to exceed the limits specified in 40 CFR 141”:

1. 5 picocuries per liter of radium-226 and radium-228
2. 15 picocuries per liter of alpha-emitting radionuclides (including radium-226, but excluding radon and uranium)
3. The combined concentrations of radionuclides that emit either beta or gamma radiation that would produce an annual dose equivalent to the total body or any internal organ greater than 4 millirems per year if an individual consumed 2 liters of drinking water per day.”

“Underground sources of drinking water” are defined as (§191.22)

“an aquifer or its portion which:

- (1) supplies any public water system; or
- (2) contains a sufficient quantity of ground water to supply a public water system; and
 - (i) currently supplies drinking water for human consumption; or
 - (ii) contains fewer than 10,000 milligrams of total dissolved solids per liter.”

We are not using groundwater protection requirements as criteria in the performance assessment. Therefore, we will not discuss them further.

Appendices to 40 CFR 191 provide additional guidance. The implementing agency must provide evaluations showing a reasonable expectation that a repository will comply with the quantitative requirements of Subparts B and C of 40 CFR 191. Appendix A of 40 CFR 191 specifies how to determine release limits for the Containment Requirements. Appendix B of 40 CFR 191 specifies how to determine the annual committed effective dose for the Individual Protection Requirements. Appendix C provides nonmandatory guidance for implementing the long-term performance requirements.

Appendix C of 40 CFR 191 is based on the analytical assumptions the EPA used to develop the technical basis for the numerical disposal standards. The EPA prepared Appendix C because the agency believed that it was important that the assumptions used by implementing agencies be compatible with those used by the EPA in developing the rule (EPA, 1985a, p. 38074). Appendix B of this report contains the text of 40 CFR 191 and provides background information on the development of the regulation.

In January 1995, the EPA issued a proposed *40 CFR Part 194: Criteria for the Certification and Determination of the Waste Isolation Pilot Plant's Compliance with Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes* (EPA, 1995). These criteria are being developed pursuant to the EPA's authority under the Waste Isolation Pilot Plant Land Withdrawal Act (WIPP LWA, 1992), which specifies that the EPA issue final criteria by October 30, 1994. The EPA intends to specify requirements for implementing 40 CFR 191 and to clarify compliance-related ambiguities that may exist. Because this applies to the WIPP, we will not discuss it further.

Sections 2.3.2 and 2.3.3 summarize the long-term performance requirements of 40 CFR 191, Subpart B, based both on the requirements as stated and on the guidance provided in Appendix C of the rule.

2.3.2 Containment Requirements

The primary objective of Subpart B is "to isolate most of the wastes from man's environment by limiting long-term releases and the associated risks to populations" (EPA, 1985a, p. 38070). This objective is reflected quantitatively in the Containment Requirements (§191.13):

"Disposal systems for spent nuclear fuel or high-level or transuranic radioactive wastes shall be designed to provide a reasonable expectation, based on performance assessments, that the cumulative releases of radionuclides to the accessible environment for 10,000 years after disposal from all significant processes and events that may affect the disposal system shall:

1. Have a likelihood of less than one chance in 10 of exceeding the quantities calculated according to Table 1 (Appendix A [of 40 CFR 191]), and
2. Have a likelihood of less than one chance in 1,000 of exceeding ten times the quantities calculated according to Table 1 (Appendix A)."

The Containment Requirements are explicitly quantitative and probabilistic; they place numerical limits not on cumulative releases, but on *likelihoods* that cumulative releases of radioactivity to the environment over a 10,000-yr period will exceed certain release values computable from formulae given in Appendix A of 40 CFR 191.

Disposal System. "Disposal system" is defined in 40 CFR 191 to mean "any combination of engineered and natural barriers that isolate...radioactive waste after disposal" (§191.12). Additionally,

"'barrier' means any material or structure that prevents or substantially delays movement of water or radionuclides toward the accessible environment. For example, a barrier may be a geologic structure, a canister, a waste form with physical and chemical characteristics that significantly decrease the mobility of radionuclides, or a material placed over and around waste, provided that the material or structure substantially delays movement of water or radionuclides" (§191.12).

The disposal system is the combination of the engineered barriers of the repository/shaft system and the natural barriers of the disposal site that isolate the wastes from the accessible environment. Engineered barriers can be seals and backfill in the emplacement facilities, and plugs in boreholes. Engineered modifications to the repository design can include making the waste itself form a barrier. Natural barriers are the subsurface geologic and hydrologic systems within the controlled area that inhibit release and migration of hazardous materials. Barriers are not limited to the examples given in the regulation's definition, nor are those examples mandatory. As recommended by the EPA in Appendix C, "...reasonable projections for the protection expected from all of the engineered and natural barriers...will be considered" (EPA, 1985a, p. 38088).

Performance Assessment. Quantitatively evaluating compliance with the Containment Requirements requires a performance assessment, which has specific meaning within 40 CFR 191:

"'Performance assessment' means an analysis that: (1) identifies the processes and events that might affect the disposal system; (2) examines the effects of these processes and events on the performance of the disposal system; and (3) estimates the cumulative releases of radionuclides, considering the associated uncertainties, caused by all significant processes and events. These estimates shall be incorporated into an overall probability distribution of cumulative release to the extent practicable" (§191.12).

2. Regulatory Criteria for Radioactive-Waste Repositories

The EPA expects that implementing agencies will make extensive use of mathematical models in the course of a performance assessment:

"The [EPA] believes that the implementing agencies must determine compliance with §191.13 [and] 191.15...of Subpart B by evaluating long-term predictions of disposal system performance. ...In making these various predictions, it will be appropriate for the implementing agencies to make use of rather complex computational models, analytical theories, and prevalent expert judgment relevant to the numerical predictions. ...In fact, sole reliance on these numerical predictions to determine compliance may not be appropriate; the implementing agencies may choose to supplement such predictions with qualitative judgments as well" (EPA, 1985a, p. 38088).

In other words, predictions made with numerical models are to be used as only part of the implementing agency's argument that the disposal system meets 40 CFR 191. However, the EPA clearly intends these predictions to be more than simple "point estimates" of releases of radioactivity by the disposal system. In the Containment Requirements, there is frequent mention of the need to account for all uncertainties that may rise in modeling the system's behavior, and a way of quantitatively presenting those uncertainties is proposed:

"...whenever practicable, the implementing agency will assemble all of the results of the performance assessments to determine compliance with §191.13 into a 'complementary cumulative distribution function' that indicates the probability of exceeding various levels of cumulative release. When the uncertainties in parameters are considered in a performance assessment, the effects of the uncertainties considered can be incorporated into a single such distribution function for each disposal system considered" (EPA, 1985a, p. 38088).

Inclusion of the expression "all significant processes and events" in the Containment Requirements indicates that performance must be determined for both undisturbed and possible disturbed future states of the disposal system. The necessity of identifying the possible future states is the justification for including scenario development in performance assessments. For human intrusion, only inadvertent—not purposeful—intrusion needs to be considered. The EPA reasoned that only future states that helped to distinguish between sites were necessary to consider.

With the minor modification of adding a water withdrawal well to provide a potential pathway for radionuclides to reach humans, the performance-assessment methodology developed for the Containment Requirements can be used to assess compliance with undisturbed performance for the Individual Protection Requirements (discussed in the subsection, "Individual Protection Requirements.")

Human Intrusion. Determining compliance with 40 CFR 191 requires performance assessments that include the probabilities and consequences of disruptive events. Appendix C of 40 CFR 191 indicates that "inadvertent and intermittent intrusion by exploratory drilling for resources...can be the most severe intrusion scenario assumed by the implementing agencies" (EPA, 1985a, p. 38089). The EPA gives specific guidance in Appendix C of 40 CFR 191 for considering inadvertent human intrusion.

The EPA specifies in Appendix C of 40 CFR 191 that "the likelihood of such inadvertent and intermittent drilling does not need to be considered greater than 30 boreholes per square kilometer of repository area per 10,000 years for geologic repositories in proximity to sedimentary rock formations, or more than 3 boreholes per square kilometer per 10,000 years for repositories in other geologic formations" (EPA, 1985a, p. 38089). In addition, the implementing agency can assume that the consequences of inadvertent drilling are no more severe than (1) direct release to the land surface of all groundwater in the repository that would promptly flow through the newly created borehole due to natural lithostatic pressure and (2) creation of a groundwater flow path with permeability typical of a borehole filled by soil or gravel that would normally settle into an open hole over time (*ibid.*).

Reliance on future active institutional control is limited in that "performance assessments...shall not consider any contributions from active institutional controls for more than 100 years after disposal" (§191.14[a]). An additional requirement, however, is that "disposal sites shall be designated by the most permanent markers, records, and other passive institutional controls practicable to indicate the dangers of the wastes and their location" (§191.14[c]). The possibility of inadvertent human intrusion must be considered and the use of passive institutional controls to deter intrusion should be "taken into account" in performance assessments. The EPA assumes that passive institu-

tional controls should "...reduce the chance of inadvertent intrusion compared to the likelihood if no markers and records were in place" (EPA, 1985a, p. 38080).

The EPA indicates in Appendix C of 40 CFR 191 that, as long as passive institutional controls "endure and are understood," they can be assumed to deter "systematic or persistent exploitation" of the disposal site, and furthermore, "can reduce the likelihood of inadvertent, intermittent human intrusion" to a degree to be determined by the implementing agency, although the possibility of inadvertent intrusion cannot be eliminated (EPA, 1985a, p. 38088).

Uncertainties. The EPA recognizes in the 1985 preamble to 40 CFR 191 that "standards must be implemented in the design phase for...disposal systems because active surveillance cannot be relied upon" over the long time of interest (EPA, 1985a, p. 38070). The EPA further notes that "standards must accommodate large uncertainties, including uncertainties in our current knowledge about disposal-system behavior and the inherent uncertainties regarding the distant future" (ibid.). The definition of performance assessment in 40 CFR 191 requires "considering the associated uncertainties" (§191.12).

"Uncertainties in parameters" are the only source of uncertainty specifically identified in 40 CFR 191 (EPA, 1985a, p. 38088). Performance-assessment methodologies recognize uncertainties in several categories of parameters (see Chapter 3). In many aspects of data collection, the professional judgment of an analyst with expertise in the area of investigation often enters into the scientific process. For example, selection of methods to collect data, interpretation of data, development of conceptual models, and selection of model parameters all require professional analysis and judgment. The analyst's final data set is based on available data, the intended use of the parameter in the computational model, the behavior of analogous systems, and the analyst's own expert judgment.

Formal expert judgment may be considered for some parameters or models identified as being important in cases where significant uncertainty exists in the available data and conceptual models, and directly applicable experimental or field data cannot be practicably obtained (Trauth et al., 1992; 1993). In these instances, formal elicitation can provide probability distributions for model parameters. These distributions can be used to provide guidance until experimental or field data become available, or, in those cases where direct acquisition of data is impossible or unrealistic, the elicited distributions can form part of the basis for compliance evaluation. Expert panels may also be used to provide independent evaluation.

Quality assurance (QA) procedures may be used for reducing uncertainty in various aspects of performance assessments. Procedures for assuring the quality of analysis results can be provided for data, software, analysis, elicitation of judgments from expert panels, and documentation (Rechard et al., 1991; 1992a; 1992b).

Release Limits. Appendix A of 40 CFR 191 establishes release limits for all regulated radionuclides. Table 1 in Appendix A gives the limit for cumulative releases to the accessible environment for 10,000 years after disposal for each radionuclide per unit of waste. Note 6 to Table 1 of the appendix describes the manner in which the release limits are to be used to determine compliance with the Containment Requirements. For each radionuclide released, the ratio of the estimated cumulative release to the release limit for that radionuclide must be determined; ratios for all radionuclides are then summed for comparison to the requirements of §191.13(a):

$$R = \sum_{i=1}^{nR} \left(\frac{Q_i}{L_i} \right)$$

where

R = the summed normalized release to the accessible environment.

nR = the number of radionuclides used in the analysis.

Q_i = the cumulative release (in Ci) of radionuclide i to the accessible environment during the 10,000-yr period following closure of the repository.

L_i = the release limit (in Ci) for radionuclide i given in Table 1, Appendix A of 40 CFR 191.

Thus, the quantity of a radionuclide that may be released depends on the quantities of all other radionuclides projected to be released, but cannot exceed its own release limit. The summed normalized release cannot exceed 1 for

2. Regulatory Criteria for Radioactive-Waste Repositories

probabilities greater than 0.1 and cannot exceed 10 for probabilities greater than 0.001, but less than 0.1. Potential releases estimated to have probabilities less than 0.001 are not limited (§191.13[a]).

An important aspect of the release limits is the waste unit factor (f_w) for limits (L_i). As more waste activity (in Ci) is placed in the repository, more radionuclides can be released legally, corresponding to the idea that more statistical deaths occur from unmined uranium ore as the volume included in the theoretical calculations increases. Thus, placing more waste into a repository can help a repository meet the release limits provided the waste has physical characteristics that reduce the overall release rate, such as better waste packaging or waste form. However, a difficulty occurs from the ratioing of permitted releases to the amount of activity in the repository. It is difficult to assess a priori the influence of adding a new or processed waste type to a repository if the added activity is significant and the mix of radionuclides is substantially different from the average waste type; the full release calculation must be redone.

Compliance Assessment. The results of the performance assessment for §191.13(a) are expected to be incorporated, to the extent practicable, into an overall probability distribution of cumulative release. In Appendix C of 40 CFR 191, the EPA assumes that, whenever practicable, results can be assembled into a single complementary cumulative distribution function (CCDF) that indicates the probability of exceeding various levels of summed normalized cumulative releases (EPA, 1985a, p. 38088) (Figure 2-5).

In the Containment Requirements, only two limit points are specified (i.e., the probabilities of exceeding 1 and 10 are required to be less than 0.1 and 0.001, respectively); however, to improve readability, on most graphs that compare a calculated CCDF to the limiting points, limiting lines connect these points (Figure 2-5).

Descriptions of a procedure for performance assessments based on the construction of a CCDF can be found in these cited reports (Pepping et al., 1983a; Hunter et al., 1986; Cranwell et al., 1987, 1990; Campbell and Cranwell, 1988; Rechard, 1989; Helton, 1993). The construction of CCDFs follows from the development of scenario probabilities and the calculation of scenario consequences. Further, the effects of different types of uncertainties can be shown by constructing families of CCDFs and then reducing each family to a single CCDF.

Figure 2-5. Complementary cumulative distribution function (CCDF) illustrating compliance with the Containment Requirements.

1 *"Reasonable Expectation" of Compliance.* As stated in §191.13(b),
 2

3 "Performance assessments need not provide complete assurance that the requirements of [§191.13(a)] will be
 4 met. Because of the long time period involved and the nature of the events and processes of interest, there will
 5 inevitably be substantial uncertainties in projecting disposal system performance. Proof of the future perfor-
 6 mance of a disposal system is not to be had in the ordinary sense of the word in situations that deal with much
 7 shorter time frames."
 8
 9

10 For §191.13(a), the EPA assumes that a single CCDF will incorporate all uncertainty (EPA, 1985a, p. 38088).
 11 The Containment Requirements (§191.13[a]) state that, based upon performance assessments, releases shall have
 12 probabilities that do not exceed specified limits. Appendix C of 40 CFR 191 states that "the [EPA] assumes that a dis-
 13 posal system can be considered to be in compliance with §191.13 if this single distribution function meets the
 14 requirements of §191.13(a)" (EPA, 1985a, p. 38088). Additional wording in §191.13(a) is that "...what is required is
 15 a reasonable expectation, on the basis of the record before the implementing agency, that compliance with 191.13(a)
 16 will be achieved."
 17
 18
 19
 20

21 **2.3.3 Individual Protection Requirements** 22 23

24 The Individual Protection Requirements in the 1993 rule state that "for 10,000 years after disposal, undisturbed
 25 performance of the disposal system shall not cause the annual committed effective dose received through all potential
 26 pathways from the disposal system, to any member of the public in the accessible environment to exceed 15 mil-
 27 lirems (150 microsieverts)" (§191.15[a]).
 28
 29

30 The methodology developed for assessing compliance with the Containment Requirements can be used to esti-
 31 mate doses as specified by the Individual Protection Requirements. One of the products of scenario development for
 32 the Containment Requirements is a base-case scenario that describes undisturbed conditions. The undisturbed perfor-
 33 mance of the repository is its design-basis behavior, including variations in that behavior resulting from uncertainties
 34 in the 10,000-year performance of natural and engineered barriers, as defined in §191.12:
 35
 36

37 "'Undisturbed performance' means the predicted behavior of a disposal system, including consideration of the
 38 uncertainties in predicted behavior, if the disposal system is not disrupted by human intrusion or the occurrence
 39 of unlikely natural events."
 40
 41

42 Undisturbed performance can be understood to mean that uncertainties in such repository features as engineered
 43 barriers (seals and plugs) must be specifically included in the analysis of the predicted behavior. Human intrusion
 44 means any human activity other than those directly related to repository characterization, construction, operation, or
 45 monitoring. The effects of intrusion are specifically excluded from the undisturbed-performance analysis.
 46
 47

48 The EPA states that the implementing agency is required to provide a "reasonable expectation" that compliance
 49 with the Individual Protection Requirements will be achieved (§191.15[c]). In addition, the EPA assumes in Appen-
 50 dix C of 40 CFR 191 that compliance with the Individual Protection Requirements "can be determined based upon
 51 best estimate predictions" rather than a probabilistic analysis. Thus, according to the EPA, when uncertainties are
 52 considered, only "the mean or median of the appropriate distribution, whichever is higher," need fall below the limits
 53 (EPA, 1985a, p. 38088).
 54
 55
 56
 57

58 **2.4 Overview of NRC's Regulation, 10 CFR 60** 59 60

61 The NRC's 10 CFR 60 differs from 40 CFR 191 in that it emphasizes the individual components of a system
 62 rather than the performance of the repository system as a whole as 40 CFR 191 does. Congress has stated that 10
 63 CFR 60 will have to be revised to be consistent with new regulations promulgated under the mandate of the Energy
 64 Policy Act, 1992.
 65
 66

2. Regulatory Criteria for Radioactive-Waste Repositories

When 40 CFR 191 was originally promulgated, the accompanying Supplementary Information in the *Federal Register* explained the relationship between 40 CFR 191 and 10 CFR 60 (EPA, 1985a, p. 38067):

"The Nuclear Regulatory Commission (NRC) and the DOE are responsible for implementing [40 CFR 191]. The NRC has already promulgated procedural and technical requirements in 10 CFR Part 60 for disposal of high-level wastes in mined geologic repositories.... The NRC will obtain compliance with 40 CFR Part 191 for disposal of all high-level wastes by issuing licenses to the DOE, in accordance with 10 CFR Part 60, at various steps in the construction and operation of a repository. Both NRC's 10 CFR Part 60 and DOE's 10 CFR Part 960 incorporate the standards the [EPA] is promulgating today as the overall performance requirements for a geologic repository. Both of these other rules were designed in concert with EPA's ongoing development of 40 CFR Part 191. However, both the NRC and DOE must now review these regulations to determine what specific changes will be needed to properly implement the final version of 40 CFR Part 191."

This text suggests that there is a hierarchy in the two regulations, with 40 CFR 191 establishing the intent and limitations for the regulation of nuclear waste repositories. Following from this hierarchy is the basic assumption that 10 CFR 60, as an implementing regulation, must not be in conflict with the regulation it is intended to implement. The following discussion of some of the most important points related to long-term performance assessments, highlights those areas in which there is currently conflict. This chapter was organized so that 40 CFR 191 was discussed first, as the regulation with primacy. The implementing regulation, 10 CFR 60, is discussed in the following sections.

2.4.1 NRC's Regulations for Radioactive-Waste Disposal

The EPA regulations establish standards for the disposal system as a whole to protect the accessible environment. However, the NRC is responsible for ensuring that a DOE disposal system for commercially generated spent fuel and high-level radioactive waste meets the requirements in EPA's 40 CFR 191. In June 1983, the NRC promulgated *10 CFR 60—Disposal of High Level Radioactive Wastes in Geologic Repositories* (NRC, 1983a). The NRC anticipated the promulgation of the EPA standard and "implemented" it by incorporating it into the agency's regulations. Yet the NRC also established minimum requirements for the engineered and geologic barriers subsystems of the disposal system (treating the disposal system similar to a nuclear reactor) that required compliance calculations (BRWM, 1992, p. 7). The requirements are stringent—a period for substantially complete containment of radionuclides by the waste packages (may vary from a minimum of 300 yr to a maximum of 1000 yr); a maximum engineered barrier release rate (1×10^{-5} /yr of the 1000 yr inventory after the containment period for any radionuclide released at a rate greater than 0.1% of the calculated total release rate limit); and a minimum groundwater travel time from the repository to the accessible environment (1000 yr) for the geologic barrier. Thus, the requirements for compliance with 10 CFR 60 potentially require the implementing agency to have a much more thorough understanding of the engineered subsystems than for 40 CFR 191 to show compliance with 10 CFR 60. They also diminish the advantage of some sites because 10 CFR 60 requires a robust canister and waste form regardless of the geologic medium of the site. For example, according to 40 CFR 191, the favorable characteristic of halite in creeping around a waste container and entombing it could mean that the implementing agency could place less reliance on the waste container or waste form; however, according to 10 CFR 60, credit could only be taken for this characteristic in performance assessments to determine compliance with 40 CFR 191, not 10 CFR 60.[‡]

The regulation has a number of interesting aspects in addition to the above subsystem requirements. The regulation includes a statement that EPA's generally applicable standards (40 CFR 191) apply to repositories subject to 10 CFR 60 (subject to Congressional action otherwise). In conducting the required "evaluation of performance," the standard of proof is to be a "reasonable assurance" of compliance. The "evaluation of performance" is actually two evaluations—one based on "anticipated processes and events" (excludes the consideration of human intrusion) and one based on "unanticipated processes and events" (includes human activities subject to a list of conditions).

[‡] While the waste package criteria for 10 CFR 60 include the caveat that the prohibitions are operational to the extent that the physical characteristics might be detrimental to achieving the performance objectives, the waste form criteria do not include the leeway to examine whether the physical characteristics impact performance objectives. Such an absolute requirement for waste form characteristics, with a potential impact on engineered modifications, calls for further guidance as to the definitions of "solid form," "particulate waste," and "noncombustible."

Other requirements of 10 CFR 60 include detailed site characterization plans (e.g., the 6300-page plan for the proposed repository at Yucca Mountain, Nevada [U.S. DOE, 1988a]) and design of the operations area of the facility "...such that any or all of the emplaced waste could be retrieved on a reasonable schedule starting at any time up to 50 years after emplacement..." where "reasonable schedule" means in the same time devoted to originally constructing the facility and emplacing the waste. A "performance confirmation program" is required to evaluate whether natural conditions and behaviors, and engineered systems behavior, are as expected, and is intended to begin during site characterization and extend until permanent closure of the repository. NRC staff analysis of public comments on the draft version of 10 CFR 60 indicates that (NRC, 1983b, p. 34):

"Rather the Commission has adopted an approach where the retrievability option is maintained until a performance confirmation program can be completed that will allow the Commission to decide, with reasonable assurance, that permanent closure of the facility, with no further active human intervention with the emplaced wastes, will not cause an unreasonable risk to public health and safety."

Thus, monitoring is continued until a decision is made to close the repository and not to retrieve the wastes. 40 CFR 191, on the other hand, requires monitoring after disposal to detect deviations from expected performance, as long as there are "significant concerns to be addressed by further monitoring" [§191.14 (b)]. The text of 10 CFR 60 is in Appendix C of this report.

As discussed in Section 2.1.2, the *Energy Policy Act of 1992* (Energy Policy Act, 1992) requires the NRC to revise 10 CFR 60 consistent with a new EPA regulation specific to the Yucca Mountain Project based on an NAS study with Congressionally specified objectives. The NAS study is expected to be available by April 1995; promulgation of the EPA regulation for the Yucca Mountain Project would then be April 1996. Based on this schedule, revision of 10 CFR 60 probably will not occur until at least 1997.

2.4.2 Organization and Disposal of High-Level Radioactive Wastes in Geologic Repositories (10 CFR 60)

10 CFR 60 contains eight subparts, two of which, Subpart B—Licenses, and Subpart E—Technical Criteria, have the most impact on performance assessments of a potential repository and the consideration of treatment options. They are described in the sections that follow. Subpart A—General Provisions, and Subpart F—Performance Confirmation Program, are also discussed briefly. In describing Subpart B of 10 CFR 60, it is important to note that we are not doing licensing at this stage. We are emphasizing the technical criteria, not the procedural steps.

2.4.3 10 CFR 60 Subparts A, B, and F

Subpart A—General Provisions. Subpart A, in part, outlines the purpose of 10 CFR 60:

"This rule prescribes rules governing the licensing of the U.S. Department of Energy to receive and possess source, special nuclear, and byproduct material at a geologic repository operations area sited, constructed, or operated in accordance with the Nuclear Waste Policy Act of 1982."

Subpart B—Licenses. Subpart B contains provisions for a Preapplication Review (dealing with site characterization); License Applications (general information, a Safety Analysis Report, and an environmental impact statement); Construction Authorization; License Issuance and Amendment (required to "receive and possess source, special nuclear, or byproduct material at a geologic operations area"); and Permanent Closure.

Within License Applications, the required Safety Analysis Report shall contain:

"An evaluation of the performance of the proposed geologic repository for the period after permanent closure, assuming anticipated processes and events, giving the rates and quantities of releases of radionuclides to the

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accessible environment as a function of time; and a similar evaluation which assumes the occurrence of unanticipated processes and events.”

The definitions in Subpart A for Part 60 provide some guidance as to how these performance assessments are to be conducted:

“Anticipated processes and events’ means those *natural* [emphasis added] processes and events that are reasonably likely to occur during the period the intended performance objective must be achieved. ...it shall be assumed that those processes operating in the geologic setting during the Quaternary Period continue to operate...”

and

“Unanticipated processes and events’ means those processes and events affecting the geologic setting that are judged not to be reasonably likely to occur during the period the intended performance objective must be achieved, but which are nevertheless sufficiently credible to warrant consideration. ...either natural processes or events or processes and events initiated by human activities other than those activities licensed under this part.”

In developing an analysis technique to evaluate compliance with both 40 CFR 191 and 10 CFR 60, the anticipated processes and events are assumed to be equivalent with the undisturbed conditions (mentioned in 40 CFR 191). The impact of human intrusion (i.e., unanticipated processes and events) is evaluated in a separate scenario, but used in developing the final CCDF.

The remainder of the definition of “unanticipated processes and events” provides additional insights into the consideration of human intrusion:

“Processes and events initiated by human activities may only be found to be sufficiently credible to warrant consideration if it is assumed that: (1) The monuments provided for by this part are sufficiently permanent to serve their intended purpose; ... (5) relevant records are preserved, and remain accessible, for several hundred years after permanent closure.”

The Supplementary Information Published with the Final Rule indicates that the regulation:

“allows for examination of intrusion under appropriate bounding conditions. ...Its objective is to provide a means for evaluating events that are reasonably of concern, while at the same time excluding speculative scenarios that are inherently implausible.” (NRC, 1983a, p. 28199).

40 CFR 191 does not place the above limitations on the consideration of human intrusion.

Though a specific time period for the conduct of such performance assessments is not mentioned in 10 CFR 60, the 10,000-yr time period in the generally applicable standard, 40 CFR 191, is assumed to apply. Also, not mentioned is guidance specifically outlining how the performance assessments are to be conducted. While not so stated in the regulation, NRC staff analysis of public comments on the draft version of 10 CFR 60 indicates that “The Commission expects that the information considered in a licensing proceeding will include probability distribution functions for the consequences from anticipated and unanticipated processes and events” (NRC, 1983b, p. 31). A probabilistic approach is assumed in accordance with the definitions in and requirements of 40 CFR 191.

While Part 60 text requires an accounting of the “rates and quantities of releases of radionuclides to the accessible environment as a function of time,” no guidance is provided as to how this should be implemented. It is not clear whether 10,000 annual releases for each radionuclide should be displayed, or whether 5-, 50-, or 100-yr averages should be displayed. This is another inconsistency with 40 CFR 191, which requires the calculation of 10,000-yr cumulative releases with associated probabilities. It is not clear, with both regulations operational, whether both sets of information should be developed and displayed.

Subpart F—Performance Confirmation Program. This subpart requires the development and implementation of a program intended to assure that natural conditions and behaviors that were expected are borne out by data, and that engineered systems behave as expected. This program must be initiated during site characterization and continued through closure of the repository. If this monitoring program detects deviations in the conditions or behaviors in excess of what was anticipated for the evaluations, then an existing plan “for feedback and analysis of data, and implementation of appropriate action” is to become operational. The “appropriate action” may include “modifications to the design or in construction methods.” As is the case with 40 CFR 191, such a confirmatory program must not “...adversely affect the ability of the natural and engineered elements of the geologic repository to meet the performance objectives.” However, the requirements of Subpart F continue only until permanent closure (until the decision is made to close the repository), while the 40 CFR 191 requirements are necessary after disposal (i.e., after the shafts are backfilled and sealed).

2.4.4 Technical Criteria

In addition to outlining technical criteria, Subpart E describes the requirement and purpose of the criteria, as well as how the purpose can be realized:

“In particular, §60.41(c) requires a finding that the issuance of a license will not constitute an unreasonable risk to the health and safety of the public. The purpose of this subpart is to set out performance objectives and site and design criteria which, if satisfied, will support such a finding of no unreasonable risk.”

and

“While these performance objectives and criteria are generally stated in unqualified terms, it is not expected that complete assurance that they will be met can be presented. A reasonable assurance, on the basis of the record before the Commission, that the objectives and criteria will be met is the general standard that is required.”

The reasonable assurance metric is also required by §60.31(a) that operations and disposal can be undertaken “without unreasonable risk to the health and safety of the public.”

This reasonable assurance requirement is a potential conflict with 40 CFR 191, which states that a “reasonable expectation” of compliance is required:

“The containment requirements call for a ‘reasonable expectation’ that their various quantitative tests be met. This phrase reflects the fact that unequivocal numerical proof of compliance is neither necessary nor likely to be obtained. A similar qualitative test, that of ‘reasonable assurance,’ has been used with NRC regulations for many years. Although the Agency’s intent is similar, the NRC phrase has not been used in 40 CFR Part 191 because ‘reasonable assurance’ has come to be associated with a level of confidence that may not be appropriate for the very long-term analytical projections that are called for by 191.13. The use of a different test of judgment is meant to acknowledge the unique considerations likely to be encountered upon implementation of these disposal standards.” (EPA, 1985a, p. 38071).

Because of this conflict, two different sets of performance assessments may be required and this could cause problems in the collection of data and the development of codes.

All of the sections of Subpart E that are discussed below were considered in the 1994 performance assessment. However, we discuss sections 113 and 135 first because they were actually used in the 1994 performance assessment to compare performance.

Performance of Particular Barriers after Permanent Closure (§60.113). The particular criteria that must be met are provided in §60.113. Special emphasis is placed on the waste package (“the waste form and any containers, shielding, packing and any absorbent materials immediately surrounding an individual waste container”) in the earlier years (300-1000 yr) because of the high temperatures and radiation levels that exist. After the early containment

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period, the engineered barrier system ("the waste packages and the underground facility") is relied upon to contain/isolate the radioactive material. More reliance is placed on human-made components and systems to contain/isolate the radioactive material rather than on the ability of the geologic formation, although there is a criterion for the performance of the geologic setting ("geologic, hydrologic, and geochemical systems of the region in which a geologic repository operations area is or may be located").

The overall intent of the human-made components and systems in §60.113 is stated:

"Containment of HLW will be substantially complete during the period when radiation and thermal conditions in the engineered barrier system are dominated by fission product decay; and...any release of radionuclides from the engineered barrier system shall be a gradual process which results in small fractional releases to the geologic setting over long times."

These goals are to be met by mandating the performance of both waste packages and the overall engineered barrier system by means of the containment period and the release rate, respectively.

Containment Period. The performance of the waste package is mandated by the following text:

"Containment of HLW within the waste packages will be substantially complete for a period to be determined by the [NRC]...provided, that such period shall be not less than 300 years nor more than 1,000 years after permanent closure of the geologic repository;"

Unfortunately, the term "substantially complete" is not defined and there is no way of determining what level of releases would constitute isolation that was not "substantially complete." In addition, with no guidance as to how the period of time will be determined, a repository program must communicate with the NRC for the defining of the containment period.

Release Rate.

"The release rate of any radionuclide from the engineered barrier system following the containment period shall not exceed one part in 100,000 per year of the inventory of that radionuclide calculated to be present at 1,000 years following permanent closure,...provided, that this requirement does not apply to any radionuclide which is released at a rate less than 0.1% of the calculated total release rate limit. The calculated total release rate limit shall be taken to be one part in 100,000 per year of the inventory of radioactive waste, originally emplaced in the underground facility, that remains after 1,000 years of radioactive decay."

The release rate for a single radionuclide (an individual release rate) must be calculated for all radionuclides expected to be present after the containment period. This means that the release of daughter products is controlled, along with the release of any radionuclides originally emplaced that have not completely decayed. The allowable release rate for an individual radionuclide is a fraction of the inventory existing at year 1000. When the total release rate limit (for all radionuclide releases) is calculated, it is a fraction of the inventory originally emplaced that is expected to be present at year 1000, not the overall inventory at year 1000. This means that the release of daughter products is used to calculate the total release, yet the calculation of the release rate limit does not include the incorporation of the inventory of daughter products at year 1000.

The allowable release rate per year for any radionuclide expected to be present after the containment period is:

$$\dot{C}_{(i)} \equiv \left\{ \frac{C_{(i)}}{C_i} \right\}_{t=1000 \text{ years}} / 100,000$$

where $C_{(i)}$ is the quantity of a particular radionuclide (originally emplaced in the repository) that is present at year $t = 1000$; and where C_i is the summation of all such radionuclides ($i = 1, \dots, n$). (Recall from the indicial notation that a "()" around a subscript means no summation.)

Since the containment period may theoretically be any length of time from 300 to 1000 years, there may be some difficulties if the containment period is set at something like 300 years. Releases during the period of high radiation levels and rapid radioactive decay will be governed by the inventory remaining at year 1000, which should be rather small.

The lack of a definition for "substantially complete" and no consideration of the release rate from the engineered barrier system prior to the end of the containment period leaves a gap in what the consequences are if any radionuclides, however small in quantity, are expected to be released from the engineered barrier system during that period.

Pre-Waste-Emplacement Groundwater Travel Time. The ability of the geologic formation to contribute to the isolation of the radioactive material is counted only in terms of the groundwater travel time, rather than considering other possible mechanisms for isolation:

"The geologic repository shall be located so that pre-waste-emplacment groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1,000 years..."

Criteria for the Waste Package and its Components (§60.135). The waste package and the waste form have to meet specific requirements in addition to meeting the above criteria based on their performance.

"Packages for HLW shall be designed so that the in situ chemical, physical, and nuclear properties of the waste package and its interactions with the emplacement environment do not compromise the function of the waste packages or the performance of the underground facility or the geologic setting."

Specifically:

"The waste package shall not contain explosive or pyrophoric materials or chemically reactive materials in an amount that could compromise the ability of the underground facility to contribute to waste isolation or the ability of the geologic repository to satisfy the performance objectives."

and

"The waste package shall not contain free liquids in an amount that could compromise the ability of the waste packages to achieve the performance objectives relating to containment of HLW..."

Specific criteria exist for the waste form, in that it must meet the following criteria:

"All such radioactive wastes shall be in solid form and placed in sealed containers. ...Particulate waste forms shall be consolidated (for example, by incorporation into an encapsulating matrix) to limit the availability and generation of particulates. ...All combustible radioactive wastes shall be reduced to a noncombustible form unless it can be demonstrated that a fire involving the waste packages containing combustibles will not compromise the integrity of other waste packages, adversely affect any structures, systems, or components important to safety, or compromise the ability of the underground facility to contribute to waste isolation."

The definition of "important to safety" is a relatively near-term concern, and thus operational aspects of repository performance are addressed with long-term radionuclide isolation/containment:

"...essential to the prevention or mitigation of an accident that could result in a radiation dose to the whole body, or any organ, of 0.5 rem or greater at or beyond the nearest boundary of the unrestricted area at any time until the completion of permanent closure."

Criticality. 10 CFR 60 is silent as to criticality occurring after closure of the repository. The only mention of criticality is in Section 60.131, "General design criteria for the geologic repository operations area". Paragraph (b)(7) adopts standard criticality control during operations similar to nuclear power plants, requiring two unlikely changes

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1 in conditions that prevent criticality under normal conditions and a five percent margin of safety on the effective mul-
2 tiplication factor (explained in Chapter 10). It is important to note that this criticality control applies only during
3 operation of the repository, not post-closure.
4

5
6 *Performance of the Geologic Repository Operations Area Through Permanent Closure (§60.111).* One aspect of
7 the regulation that must be considered in the design and construction of a proposed repository has to do with retriev-
8 ability of waste:
9

10 "...the geologic repository area shall be designed so that any or all of the emplaced waste could be retrieved on a
11 reasonable schedule starting at any time up to 50 years after waste emplacement operations are initiated,"
12

13
14 and

15
16 "For purposes of this paragraph, a reasonable schedule for retrieval is one that would permit retrieval in about the
17 same time as that devoted to construction of the geologic repository operations area and the emplacement of
18 wastes."
19

20
21 This is in conflict with 40 CFR 191 which, although stating that removal of wastes must not be precluded, also states
22 in the accompanying Supplementary Information (EPA, 1985a, p. 38082) that:
23

24
25 "The intent of this provision was not to make recovery of waste easy or cheap, but merely possible in case some
26 future discovery or insight made it clear that the wastes needed to be relocated. EPA reiterates the statement in
27 the preamble to the proposal that *any* [emphasis in original] current concept for a mined geologic repository
28 meets this requirement *without* [emphasis in original] any additional procedures or design features. ...To meet
29 this assurance requirement, it only need be technologically feasible (assuming current technology levels) to be
30 able to mine the sealed repository and recover the waste—albeit at substantial cost and occupational risk.
31 ...Therefore, this provision should not have any effect upon plans for mined geologic repositories. Rather, it is
32 intended to call into question any other disposal concept that might not be so reversible...."
33
34

35
36 While the assurance requirements as written in 40 CFR 191 do not apply to facilities regulated by the NRC, Part 60
37 appears to be in conflict with the intent of Part 191, which is counter to the agreement between EPA and NRC (EPA,
38 1985a, p. 38072):
39

40
41 "The final rule incorporates the five remaining assurance requirements plus the requirement for long-term moni-
42 toring, but it makes them applicable only to disposal facilities that are not regulated by the NRC. ...However,
43 the two agencies have agreed to resolve this issue by having the [NRC] modify 10 CFR Part 60 where necessary
44 to incorporate the intent of the assurance requirements, rather than having them included in 40 CFR Part 191 for
45 NRC-licensed disposal facilities. ...EPA has provided NRC with all of the comments received on the assurance
46 requirements during the 40 CFR Part 191 rulemaking, and the [EPA] will participate in the NRC rulemaking to
47 facilitate our objective of having the intent of all of the assurance requirements embodied in Federal regulation."
48
49

50 Requirements in 10 CFR 60 may specify design components that could be very costly and that are inconsistent with
51 the intent in 40 CFR 191.
52

53
54 *Overall System Performance Objective for the Geologic Repository After Permanent Closure (§60.112).* Subpart
55 E also establishes the applicability of EPA generally applicable standards (i.e., 40 CFR 191):
56

57
58 "The geologic setting shall be selected and the engineered barrier system and the shafts, boreholes and their seals
59 shall be designed to assure that releases of radioactive materials to the accessible environment following perma-
60 nent closure conform to such generally applicable environmental standards for radioactivity as may have been
61 established by the Environmental Protection Agency with respect to both anticipated processes and events and
62 unanticipated processes and events."
63

64
65 The above text explicitly states that 40 CFR 191 should be the driving force in the design of the repository in order
66 that compliance with the probabilistic release limits in §191.13 can be shown. Together with the text from the Sup-

plementary Information provided with the 1985 promulgation of 40 CFR 191 (EPA, 1985a, p. 38067, as discussed earlier), 40 CFR 191 is established as the primary regulation governing high-level waste repositories, with 10 CFR 60 intended as a regulation to implement 40 CFR 191.

Siting Criteria (§60.122). "A geologic setting shall exhibit an appropriate combination of the [favorable] conditions specified in paragraph (b) of this section so that, together with the engineered barrier system, the favorable conditions present are sufficient to provide reasonable assurance that the performance objectives relating to isolation of the waste will be met. ...If any of the potentially adverse conditions specified in paragraph (c) of this section is present, it may compromise the ability of the geologic repository to meet the performance objectives relating to isolation of the waste."

"...not to affect significantly the ability of the geologic repository to meet the performance objectives relating to isolation of the waste, or the effect of the potentially adverse human activity or natural condition is compensated by the presence of a combination of the favorable characteristics so that the performance objectives relating to isolation of the waste are met..."

The potentially adverse conditions include resources within the site, previous mining for resources within the site, previous drilling for any reason within the site, and the potential for gaseous radionuclides to migrate from the repository to the accessible environment. The allowance for the balancing of favorable and potentially adverse conditions in the consideration of a possible site is similar to the language in 40 CFR 191 (EPA, 1985a, p. 38069):

"The wording in the proposed rule would have ruled out sites with a significant possibility of being considered for resources exploration in the future. The final rule revises this requirement to allow use of sites with some resource potential if they have other significant advantages compared to potential alternative sites."

2.5 Hazardous-Waste Disposal Regulations

The *Resource, Conservation, and Recovery Act of 1976* (RCRA) and subsequent amendments (e.g., *Hazardous and Solid Waste Amendments of 1984* [HSWA]) provide for management of waste contaminated with hazardous chemicals. The EPA regulations implementing the requirements of these acts are contained in 40 CFR 224 through 40 CFR 281. The statute and associated EPA implementing regulations are complex; the manner in which their provisions will influence fuel- and waste-treatment options and eventual disposal is currently uncertain. Furthermore, a more important fundamental issue is whether consideration of requirements in the RCRA would increase protection to human health and the environment beyond requirements in the two primary regulations for long-term disposal of radioactive waste, 40 CFR 191 and 10 CFR 60. Some points for consideration follow, but no final conclusions have been reached.

Spent Nuclear Fuel Classification. Spent nuclear fuel has not yet been formally classified as waste by the DOE; thus, the EPA waste management regulations have not been applied to this material. However, spent fuel has been included in the "180-day report" mandated by the *Federal Facility Compliance Act of 1992* (FFCA, 1992) as part of the DOE's mixed waste inventory, and spent fuel would likely be declared as waste prior to disposal in a repository.

RCRA Hazardous Waste Characteristics. Hazardous-waste characteristics are usually not thought to be present in spent nuclear fuel and solidified liquid high-level waste. However, RCRA hazardous-waste characteristics potentially exhibited by spent fuel and high-level waste include reactivity, toxicity for metals, and corrosivity.

In some spent fuel, sodium metal was used to bind fuel to the cladding. This fuel might be considered reactive. Also, although very slow, reaction of water with the silicon carbide coating on graphite fuels can form acetylene gas. Finally, the uranium and thorium carbide microspheres, once the silicon carbide coating fails, can react quickly to form acetylene gas.**

** Similarly, recall that all gas produced from anoxic corrosion of stainless steel canisters is hydrogen gas.

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Certain spent fuel contains toxic metals listed in 40 CFR 161.14, including (1) chromium in stainless steel in cladding and assembly components, (2) stable fission products such as barium, cadmium, selenium, and silver; and (3) metals in failed fuel such as control rods fused with fuel from the Three Mile Island reactor. Because of low concentrations, the first two sources probably would not fail tests specified by the EPA for evaluating the amount of hazardous material that may leach out if disposed of directly, while the third source (not included in this performance assessment) might.^{††}

Liquid high-level waste stored at INEL is acidic and thus corrosive.^{‡‡}

RCRA-Listed Materials. In the past, chemicals currently classified as hazardous were possibly used in laboratories handling radioactive material ("hot labs") at chemical plants. Waste from these labs was routinely placed in stainless steel tanks storing liquid radioactive waste. Thus, very small quantities of RCRA-listed material can be present in the liquid and possibly solidified high-level waste.

Compliance Strategy. In performing assessments for a potential repository, an approach to responding to the RCRA requirements could be to follow the example of the DOE's proposed TRU-waste repository (the Waste Isolation Pilot Plant in New Mexico). The approach is to petition for a "no-migration" variance to the land-disposal restrictions (40 CFR 268.6). This petition would allow hazardous chemicals to be disposed of in the repository for the maximum length of time allowed in the permit, with renewals as necessary (WEC, 1989). This approach is taken in lieu of using the "best demonstrated available technology" (BDAT) currently defined by the EPA for radioactive waste co-contaminated with hazardous chemicals listed in EPA 40 CFR 261. The petition for the variance requires monitoring and predictive calculations, but the rigor and stochastic nature required of the calculations is currently being negotiated.

In contrast, any treatment plant that conditioned spent fuel or high-level waste would need to consider the RCRA requirements. For example, the state of Idaho has already issued a Notice of Noncompliance under RCRA for sodium-bearing waste stored at INEL, and the DOE has entered into a consent order requiring removal of the waste from the stainless-steel tanks by the year 2015.

^{††} Inclusion of lead as an internal backfill and/or container layer might also cause difficulties with the RCRA regulations, depending on EPA's interpretation of its use as related to disposal.

^{‡‡} High-level liquid wastes stored at INEL are unique within the DOE's weapons complex because they are stored in an acidic form. Although this type of storage requires stainless steel storage tanks enclosed in concrete vaults, the decision to store waste in acidic form was based on the desire to (1) maintain radionuclides in solution (as opposed to neutralized sludge at the bottom of less expensive, carbon steel tanks), and (2) greatly reduce the likelihood of precipitates of highly enriched uranium.

3. PA Methodology Overview

M. S. Tierney

3.1 Introduction

The U.S. Environmental Protection Agency's (EPA's) guidance and intentions concerning the nature and purpose of performance assessment (see Chapter 2) suggests that PA is ideally a *stochastic simulation* (Section 3.2.4) of possible long-term behaviors of a real system with a computer-implemented mathematical model of that system. In this respect, performance assessment is similar to other large-scale simulations (e.g., the *Reactor Safety Study* [Rasmussen, 1975]) that have been used by federal agencies in the past to explore policy options and develop regulations. Performance assessments of systems for the disposal of radioactive and toxic wastes may nevertheless differ from most simulations with "regulatory models" (Morgan et al., 1990, p. 292) in two significant and related ways: the way results of a performance assessment are to be used; and the nature of the real system that is being simulated.

In contrast with past simulations with federally sponsored models, PA results are ultimately used to test compliance of a real system with an existing environmental standard, not merely to gain insight into the behavior of the system with the purpose of discovering a rational basis for new standards. Furthermore, a quantitative treatment of uncertainty in PA calculations is not merely good analytical practice but is mandated by the explicitly probabilistic statement of the Standard in which all results are to be combined in an "overall probability distribution" whenever practicable. As will be seen later, such a quantitative treatment of uncertainty forces the development of two categories of models of the same system: the usual, deterministic phenomenological models (called "consequence" models in PA; Section 3.2.1), and probability models (Section 3.2.3) that can provide quantitative estimates of the degree of uncertainty associated with parameters that specify the possible configurations of the consequence models.

The problems arising from direct use of PA results in testing compliance and a mandated quantitative treatment of uncertainty are compounded by the nature of the focal system in PA: geologic waste-disposal systems are built up largely from natural components (as opposed, for example, to the man-made components of a nuclear reactor), the physical and chemical characteristics of which are usually inhomogeneous and distributed in space and time. There is little published work on efficient methods for conducting sensitivity and uncertainty analyses of such distributed-parameter systems; objective methods for the assignment of the parametric uncertainty associated with such systems are also lacking. Indeed, in building methodologies for PA, investigators have in the past drawn heavily upon ideas and analytical techniques developed primarily for the study of "lumped parameter" systems and have largely ignored the special needs of PA that arise from the problems mentioned above.

With the hope that a firm understanding of the structure of a PA will help in meeting PA's special needs, this overview offers a description of current PA methodologies in terms and concepts taken from the broader context in which they are imbedded, i.e., the general theory of stochastic simulation, as it is applied to the study of natural systems that may change or "fail" over long periods of time. To minimize misunderstanding among investigators with diverse backgrounds, terminology developed for PA will be maintained throughout the overview, but PA terms will be matched with their mathematical counterparts whenever possible. Discussion of each topic proceeds from generalities to specifics, and from theory to practical applications. The structure of a PA is summarized in Section 3.2, where emphasis is upon the correspondence of PA concepts such as consequence models, probability models, and performance measures, with concepts from the general theory of stochastic simulation. Section 3.3 is a technical treatment of certain topics of special interest to PA practitioners; in particular, the confusing topic of "scenarios" is treated.

Examples from the performance assessment described in this report became available too late to use in this Methodology Overview; consequently, I have kept the applications and examples from an earlier draft of this chapter: these are from an assessment of the performance of the Waste Isolation Pilot Plant (WIPP), a research and development facility located in southeastern New Mexico for the purpose of demonstrating safe disposal of defense-generated transuranic wastes (WIPP PA Division, 1991a, 1991b; WIPP PA Department, 1992b). The reader is assured that the general methodology used for performance assessment of the system described in the present report is substan-

tially the same as that used for the WIPP PAs. Note, however, that the general approach to performance assessment used in the two PAs for Yucca Mountain (Barnard et al., 1992; Wilson et al., 1994) is very different from the methodology described in this overview and throughout the remainder of this report.

3.2 Structure of a Performance Assessment

Simulation can be defined as the study of a system or phenomenon using a *model* of that system or phenomenon. Indeed, the ideas of simulation and modeling are intimately linked since a "model" can be defined as a tentative ideational structure that is used as a testing device. Models used in simulations can take different forms: pictorial, mechanical, verbal, and mathematical. Since the advent of high-speed digital computers in the 1950s, the use of computer-implemented mathematical models for simulations of natural and engineered phenomena has become routine. In contrast with the other forms of models, a mathematical model is relatively inexpensive and has the advantages of unequivocal and testable structure and numerical output. Nevertheless, good modeling practice dictates that pictorial and verbal models be constructed prior to construction of the mathematical model; PA analysts have called these prior pictorial/verbal models "conceptual models."

The operations of a computer-implemented mathematical model can be viewed as the evaluation of a *function*, i.e., a correspondence between sets of numbers that has the form $y = f(x)$, where: $x = (x_1, x_2, x_3, \dots, x_N)$ is a point in a subset of N-dimensional Euclidean space called the domain, D_N [or *parameter space* in PA terminology, (Section 3.2.2)]; $y = (y_1, y_2, y_3, \dots, y_M)$ is a point in a subset of M-dimensional Euclidean space called the range, R_M , (or the "consequences" in PA terminology); and the notation $f(\circ)$ stands for the operations of the mathematical model [called a *consequence model* in PA terminology, [3.2.1]] that transforms parameters x into consequences y . Since the operations implicit in a function $f(\circ)$ are nowadays almost always carried out by coded programs for a digital computer, no distinction will hereinafter be made between "function" and "computer code."

3.2.1 Consequence Models

In this overview, it is assumed that all functions representing consequence models are *deterministic*; roughly speaking, this means that for each vector of input parameters, x , there is a unique vector of consequences, y . Note that not all mathematical models of the types commonly used in PA (i.e., models formulated in terms of difference, ordinary, or partial differential equations) can be expected to be deterministic. Because of extreme sensitivity of solutions to initial values or certain problem parameters, some nonlinear models used in PA work could yield different values of y for consecutive calculations that started with single value of x . Glimm (1991) calls this apparently stochastic behavior "spontaneous chaos" and distinguishes it from the case of "external" or "forced chaos" that arises when some or all of the input parameters $x_1, x_2, x_3, \dots, x_N$ are treated intentionally as *random variables*.

There has been little or no investigation of the effects of spontaneously chaotic models on the probabilistic performance measures of interest in PA. In contrast, PA studies almost exclusively employ forced chaos in the following way: the user of a deterministic model forces it to exhibit stochastic behavior among the results of consecutive runs of the model by randomly sampling the parameters for each run from predetermined probability distributions, i.e., by randomly choosing different "realizations" of the parameter sets for each consecutive run. The collection of outcomes of the consecutive runs can then be treated as a random sample (in the statistical sense) of some quantitative measures of system behavior. This procedure is called Monte Carlo simulation (see Hammersley and Handscomb, 1964; Rubenstein, 1981; Ross, 1985), which is a variant of *stochastic simulation* (3.2.4; see also Ripley, 1987). The construction of probability distributions suitable for sampling uncertain model parameters in a *stochastic simulation* can be called *probability modeling* (Section 3.2.3).

The reasons for introducing forced stochasticity in a PA consequence model are to facilitate the study of the sensitivity of model consequences to changes in the model's parameters (sensitivity analysis; see Helton et al., 1991) and to map parametric uncertainty onto uncertainty in the model's results (uncertainty analyses). In particular, uncertainty analyses can be used to form estimates of probabilistic performance measures (Section 3.2.4) such as the one that is to be compared with EPA's probabilistic standard.

A mathematical model of a system can be called "complete" or "total" if the model captures all effects or phenomena of concern to the users of the model. Total-system models are usually formed by linking submodels that capture specific effects or phenomena in a network under the control of a master ("driver") routine. The deterministic function that represents the consequences of a total-system model,

$$c = f(x), \quad (3-1)$$

can be built up by consecutive application of several functions that individually represent the outputs of models of selected system components (here called "submodels"). For $I \geq 3$ components, a calculation of a consequence $c \in R_M$ might proceed as follows:

$$y_1 = f_1(x_1), \quad y_2 = f_2(y_1, x_2), \quad y_3 = f_3(y_2, x_3), \quad \dots$$

$$c = y_I = f_I(y_{I-1}, x_I). \quad (3-2)$$

In this expression, x_i ($i = 1, 2, 3, \dots, I$) stands for the vector of free parameters that appear in the i th submodel and y_i ($i = 1, 2, 3, \dots, I$) stands for the vector of dependent variables produced by the i th submodel. The symbol f_i , ($i = 1, 2, 3, \dots, I$) stands for the function (or computer code) representing the transformations performed by the i th submodel on its input variables and free parameters to produce an output, y_i .

Excepting y_I , which is identified with the output or consequences c , of the total-system model, the dependent variables y_i should here be regarded simply as a set of intermediate variables that are generated by the i th submodel and passed as input to the $(i+1)$ st submodel. Though some of these intermediate dependent variables may be of interest to users of the model (in PA analyses, all are usually recorded during the course of a calculation), they play no direct role in determining the dimension and structure of the total-system model's parameter space D_N or consequence space R_M . The crucial role played by the submodels' free-parameter vectors, $\{x_i\}$, in determining the dimension and structure of D_N is discussed in the next section (Section 3.2.2).

In PA work, the function f_i , representing the transformations performed by the i th submodel on its input variables and free parameters, is usually a numerical solution of one or a combination of the following kinds of equations:

- a. Partial differential equations - which model dynamics and statics of continuous media and are reduced to a set of algebraic equations or ordinary differential equations in order to effect a numerical solution by finite-difference or finite-element methods.
- b. Ordinary differential equations - which may result from the reduction of a system of partial differential equations or may directly model the dynamics of a system with discrete components: e.g., a model of a pressurized brine reservoir, or the dissolution of a finite volume of waste material.
- c. Algebraic equations of the form

$$F(x_1, x_2, x_3, \dots, x_n; y) = 0$$

which may arise indirectly from equilibrium solutions of ordinary differential equations (i.e., solutions in which time $\rightarrow \infty$), or may directly express some physical relationship between parameters $(x_1, x_2, x_3, \dots, x_n)$ and dependent variables y .

Numerical solutions of these types of equations on digital computers require discretization of independent variables specifying spatial coordinates and time. Accordingly, quantities intended to represent spatially continuous model parameters or spatially and temporally continuous solutions are necessarily specified at a finite number of points on a discrete space-time grid. This fact makes reasonable an assumption implicitly made in the foregoing paragraphs: that all parameters of the i th submodel can be represented as a finite-dimensional vector x_i , and that all outputs from the i th submodel can be represented as a finite-dimensional vector y_i .

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The composite nature of total-system consequence models distilled by Expression 3-2 is here illustrated with an example taken from a WIPP preliminary performance assessment (WIPP PA Department, 1992b). Figure 3-1 shows eight submodels, named in bold capitals by the names of their implementing computer codes (Table 3-1), that WIPP project investigators have constructed and used to estimate the consequences of inadvertent drilling into the WIPP repository for radioactive wastes (labelled by "Panel" in Figure 3-1). Other important features in Figure 3-1 are the accessible-environment boundary (marked by the line supporting the drilling rig and withdrawal well *plus* the vertical dotted line on the right) and the brine reservoir at the bottom. Here, consequences are measured in two ways: (a) by the cumulative amount of radioactivity crossing the accessible-environment boundaries in a 10,000-yr period following closure of the repository; and (b) by the radiation dose incurred by humans who use water from the withdrawal well and stock pond.

Several distinct sequences of submodels (or code linkages) are shown in Figure 3-1; the sequence used in this example is one that calculates the groundwater-pathway contribution to type (a) consequences during realization of the following summary scenario (Section 3.3.1):

...one or more boreholes penetrate through a waste-filled room or drift and continue into or through a brine reservoir in the underlying Castile Formation ... radionuclides may reach the subsurface boundary of the accessible environment following long-term groundwater transport up the borehole and laterally down a potentiometric gradient in the Culebra Dolomite Member of the Rustler Formation (WIPP PA Department, 1992b).

The code linkage for this scenario takes the following form:

(SANCHO $\Rightarrow$ BRAGFLO) $\Rightarrow$ PANEL $\Rightarrow$ (GRASP-INV $\Rightarrow$ SECO2D $\Rightarrow$ SECO/TP)
 $\Rightarrow$ [summation of type (a) consequences],

Figure 3-1. Submodels used in 1992 WIPP performance assessment (adapted from Fig. 3.6, WIPP PA Department, 1992b)

Table 3-1. Selected Computer Models Used in 1992 WIPP Performance Assessment*

Model	Description
CUTTINGS	Calculates the quantity of radioactive material (in curies) brought to the surface as cuttings and cavings generated by an exploratory drilling operation that penetrates a WIPP waste panel.
BRAGFLO	Simulates multiphase flow of gas and brine through a porous, heterogeneous reservoir (a collapsed WIPP waste panel); includes gas generation by corrosion of metals and microbial action; requires that porosity of panel as a function of time be given by SANCHO.
GRASP-INV	Generates realizations of transmissivity fields in the Culebra Dolomite Member of the Rustler Formation for use in SECO2D.
PANEL	Using brine discharge from BRAGFLO, calculates discharge and integrated discharge of radionuclide mass from a collapsed and punctured WIPP waste panel through an intrusion borehole; accounts for nuclide decay chains.
SECO2D	Simulates Darcy velocity as a two-dimensional field in the Culebra Dolomite Member of the Rustler Formation; requires transmissivity fields simulated by GRASP-INV.
SECOTP	Simulates transport of dissolved radionuclides in the groundwater of the Culebra Dolomite Member of the Rustler Formation which is treated as a fractured, porous, chemically-reacting medium; requires Darcy velocity field simulated by SECO2D.
SANCHO	Simulates dynamics of closure of a WIPP waste panel as the quasistatic, large deformation, inelastic response of a two-dimensional, porous solid; accounts for gas pressure in pore space. Used in 1992 to determine average porosity of panel as a function of time and the amount of gas generated by corrosion and microbial action.

* From WIPP PA Department, 1992b.

where an arrow ($\Rightarrow$) denotes passage of dependent, auxiliary variables between submodels, and groupings of dependent submodels are enclosed in parentheses; e.g., SANCHO furnishes variables to BRAGFLO, and the combination SANCHO + BRAGFLO passes variables to PANEL. The function representing the total-system consequences (for the particular scenario described above) may therefore be developed from three functions, each of which represents a grouping of dependent submodels:

$$y_1 = f_1(x_1), \quad y_2 = f_2(y_1, x_2), \quad y_3 = f_3(y_2, x_3),$$

$$y_3 \Rightarrow [\text{summation of type (a) consequences}].$$

The vectors x_1 , x_2 , x_3 represent arrays of the free parameters appearing respectively in the groups (SANCHO + BRAGFLO), PANEL, and (GRASP-INV + SECO2D + SECOTP).

3.2.2 Parameter Space

In Section 3.2.1 it was stated without proof that the operations of a mathematical model of a system can be regarded as the evaluation of a function of the form $c = f(x)$, where x is a vector whose elements are the free parameters of the model and c is a vector whose elements are "consequences", i.e., quantities of interest to users of the model. The ideas of consequences and consequence models were treated briefly in Section 3.2.1; the focus in the present section is upon the meaning and structure of the space of free parameters appearing in a model of the complete (or total) system.

The free parameters of a total-system model are all of the numbers that must be supplied by the user of a model in order to make it run (of course, some of these numbers may be "built into" the implementing computer codes; they are nevertheless free in the sense that they are not calculated numbers and may be easily changed). These numbers may also be called the problem input or the problem's independent variables. In Section 3.2.1, the free parameters for a system comprised of I submodels were arranged as elements of I vectors, $x_1, x_2, x_3, \dots, x_I$, of possibly different dimensions. A typical vector from this collection, say the i th one, can be written as the array

$$x_i = [x_{i1}, x_{i2}, x_{i3}, \dots, x_{im(i)}],$$

showing the individual free parameters appearing in a submodel with $m(i)$ independent parameters. Each element in such an array of numbers stands for a single parameter that has a definite meaning in the context of at least one of the submodels: for example, a certain element might stand for the value of a certain material property in a specific cell of the model's spatial grid; another element might represent a dimension of some physical feature being modeled.

Note that the same parameter may be required by more than one submodel and may therefore be a common element of several of the vectors specifying the submodel parameters. These common elements are counted only once in forming the elements of the vector of free parameters of the total-system model: assuming that there are N distinct parameters, the vector of free parameters of the total system will hereinafter be displayed as

$$x = (x_1, x_2, x_3, \dots, x_N) \quad (3-3)$$

Although the order in which the elements x_n , $n = 1, 2, 3, \dots, N$, appear in array (3-3) is unimportant for purposes of theoretical description, order is obviously important when numerical values are assigned to elements and so a fixed order for the N elements in vectors like Expression 3-3 is assumed for the remainder of this overview. Given an ordering of elements and the fact that the x_n s are real numbers or integers, it is seen that x represents a point in N -dimensional Euclidean space. Since the x_n s are intended to represent real quantities that have meaning in science or engineering, there will be restrictions on the *ranges* of numbers that may be assigned to them; by allowing each element to sweep over its natural range, the vector x will sweep over a subset of N -dimensional Euclidean space that is here called *parameter space* and denoted by D_N . A vector $x \in D_N$ is called a *parameter set*.

If the reader is to fully appreciate the simplicity and power of stochastic simulation, he/she should first appreciate the broad range of possibilities for the types of quantities that can make up the elements of a parameter set. Roughly following Morgan et al. (1990, p. 50), the types of quantities that can appear as elements of a parameter set fall in at least six categories:

1. *Model constants*, e.g., precisely known constants such as Planck's constant = 6.6256×10^{-27} erg s, or $\pi = 3.14159$.
2. *Model-domain parameters*, e.g., coordinates of nodes on spatial and temporal grids; locations and dimensions of engineered features of the system.
3. *Model control parameters*, e.g., any parameter assigned by the user to control timing and accuracy of computations: number of dynamic time steps, numbers giving convergence criteria, cutoff values for certain dependent variables.

4. *Material-property parameters.* Parameters specifying magnitudes of physical or chemical properties of materials that occupy cells of a spatial grid or parts of system features; this category may also include initial and boundary conditions on submodel dependent variables.
5. *Event-and-process parameters.* This category is the time-domain counterpart of material-property parameters; it includes the number of external events of a given kind that act upon the system during a given interval on the time grid (e.g., the number of exploratory boreholes that penetrate a waste disposal compartment between 2000 and 3000 yr after closure) and the intensities of external processes that affect the system during each interval of the time grid (e.g., mean precipitation and temperature as functions of time in a region under changed climatic conditions).
6. *Indices for alternative models.* In many cases, there are several acceptable submodels of a phenomenon of interest to PA that nevertheless may differ in their influence on the results of a calculation with the total-system model. To test the influence of each alternative model, the alternatives are numbered, runs are made of the total-system model incorporating each alternative, and results are compared. Though seemingly arbitrary, the indices of the alternative models can be sensitive elements of the parameter set.

A seventh category can be added to the list above when, for purposes of uncertainty analyses, probability models (Section 3.2.3) are used to assign likelihoods to ranges of the values taken by uncertain members of the parameter set that belong to categories 4, 5, and 6.

7. *Probability-model parameters,* e.g., means, variances and correlation coefficients in analytic probability distributions for values of material-property parameters; mean rates of occurrence of events of a given kind (appearing in probability distributions for event-and-process parameters); weights assigned to the indices of alternative forms of a submodel.

Note on uncertain parameters:

An *uncertain* (or imprecisely known) *parameter* is one that cannot be assigned a single, precise value because: (a) measurements of quantities from which the parameter can be calculated are dispersed and too few in number to form a sufficiently precise estimate of the parameter using classical methods of statistics; or (b) the parameter characterizes some aspect of a hypothetical event, process, or natural feature (e.g., the number of boreholes that penetrate an underground waste repository in the 10,000-yr period following closure). Parameters in categories 1 through 3 are seldom treated as uncertain quantities; model-domain parameters are almost always chosen by the user to reflect specifications of engineered components; model control parameters may be varied at will by the user, usually within well-documented limits set by the model's creators.

On the other hand, some degree of uncertainty is always associated with material-property parameters, particularly those derived from properties of inhomogeneous, hard-to-characterize natural (as opposed to engineered) materials. Spatial inhomogeneity of geologic materials and structures, the impracticality of making a statistically significant number of measurements of most geologic quantities, and difficulties in scaling up measured properties to reference volumes appropriate for a mathematical model all dictate that subjective (Bayesian) methods be adopted for the quantitative treatment of uncertainty in category-4 parameters. The need for a Bayesian approach in quantifying the uncertainty of parameters in categories 5 and 6 is even stronger: apart from placing known, common-sense bounds on their ranges, these event-and-process parameters are not amenable to estimation by classical statistical techniques and should be regarded as truly stochastic quantities.

The usual Bayesian approach to modeling uncertainty in event-and-process parameters is to construct a probability model (Section 3.2.3) that the analyst believes will adequately represent that uncertainty, given knowledge of a few category-7 parameters. In simple terms, probability models for event-and-process parameters are invariably *conditional probability distributions* (see Feller, 1966). Treatment of uncertainty in the category-7 or probability-model parameters then requires adoption of a second level of probability models, and so on; but in practice this hierarchy of probability models is usually closed at the first level by assuming the probability-model parameters to be constants.

In more refined Bayesian methodologies (Martz and Waller, 1982), uncertainty in a parameter is quantified by first postulating a probability model (usually expressed as an analytic formula) that provides a quantitative measure of uncertainty, called the *prior distribution*, in the parameter's values in terms of a few auxiliary constants—here called category 7, or probability-model parameters; these auxiliary parameters are then fit initially with available empirical data or, in most cases, chosen by subjective judgment. In principle, further empirical or subjective information can be used to “update” the probability model and/or its constants by application of Bayes' Rule to form *posterior distributions*, which presumably reflect a better estimate of the range of uncertainty. It is an unfortunate feature of PA work that the high cost of obtaining “further empirical or subjective information” often precludes use of the more-refined Bayesian methods.

The difference between uncertain and fixed parameters in the parameter set of a total-system model can be emphasized by partitioning the parameter space, D_N , into the space of uncertain parameters, D_{Nu} , and the space of fixed parameters, D_{Nf} , i.e.,

$$D_N = D_{Nu} \cup D_{Nf}$$

and splitting the parameter set accordingly: $\mathbf{x} = (\mathbf{x}_u, \mathbf{x}_f)$. The space of uncertain parameters, D_{Nu} , is of primary interest in sensitivity analyses and stochastic simulation of system performance (Section 3.2.4); the space of fixed parameters, D_{Nf} , is of primary interest in sensitivity analyses and in the *validation* and *verification* of computational models of system components. Validation of a computational model means finding that the model predicts well-understood phenomena with accuracies deemed sufficient by the user (but note that it may not be practicable to validate PA consequence models intended to predict poorly understood or hypothetical phenomena). Verification of a computational model usually means finding that the model reliably performs its operations or transformations in precisely the ways intended by its creators. Both validation and verification may involve the users' “fine tuning” of the model's fixed parameters.

For purposes of this overview, there is no loss in generality if the space of fixed parameters is ignored and the total parameter space is restricted to the space of uncertain parameters. Thus, the notation $\mathbf{x} \in D_N$ will hereinafter mean that elements of $\mathbf{x}_u$ are chosen from the space D_{Nu} , and that elements of $\mathbf{x}_f$ remain fixed at the values assigned by the user.

The idea of uncertain parameters is further illustrated by an example from the 1991 WIPP PA (WIPP PA Division, 1991a). Consequence models used for the 1991 series of calculations employed more than 120 distinct parameters in the five categories mentioned above (including several spatially varying quantities such as formation transmissivity). A total of 45 of these parameters were deemed sufficiently uncertain to warrant the assignment of probability models; of these, 40 were material-property parameters (Table 3-2), and 4 could be classified as event-and-process parameters (Table 3-3). Not mentioned in these tables are five event-and-process parameters specifying the number of accidental penetrations of waste-disposal areas by exploratory drilling during each of five 2000-yr time intervals spanning the 10,000-yr period following closure of the site. The probability that any one of these five parameters could take values 0, 1, 2, ..., was calculated with a probability model based on the assumption that accidental drilling follows a homogeneous Poisson process (WIPP PA Division, 1991a, p. 2-7). The single probability-model parameter specifying the Poisson process, the rate constant, is mentioned in Table 3-3.

3.2.3 Probability Models

The class of uncertain model parameters introduced in Section 3.2.2 was distinguished by the model users' inability to assign to any one of its members a single, precise value for reasons of imperfect (or total lack of) information concerning the parameter's location within its natural range of values. The very nature of this kind of uncertainty, called *parametric uncertainty*, suggests that uncertain parameters be regarded as random variables (see Feller, 1966) and that parametric uncertainty be quantified by forming probability distributions for the random variables associated with each uncertain parameter. But even when there are extensive empirical data concerning ranges of values taken by a parameter and the methods of classical statistics can be employed in estimating its distribution, construction of a probability distribution for that parameter will always involve some subjective assumptions. Thus, constructing a

Table 3-2. Uncertain Material-Property Parameters of Consequence Models Used in 1991 WIPP PA Exercises (adopted from Tables 6.0-1 and 6.0-2 of WIPP PA Division, 1991b).

Material	Properties
Halite within Salado Formation	Undisturbed permeability and pore pressure.
Anhydrite layers within Salado Formation	Undisturbed permeability, porosity, pore pressure; threshold displacement pressure.
Castile Formation Brine	Initial pressure; bulk reservoir storativity.
Culebra Dolomite Member of Rustler Formation	Longitudinal dispersivity; matrix and fracture porosity; fracture spacing; matrix and fracture partition coefficients for elements Am, Np, Pu, Th and U; transmissivity field (60 equally likely realizations).
Unmodified waste form	Gas generation rates for corrosion and microbial action under inundated and humid conditions; stoichiometric coefficients for corrosive and microbial action; solubilities for nuclide charge states Am ³⁺ , Np ⁴⁺ , Np ⁵⁺ , Pu ⁴⁺ , Pu ⁵⁺ , Th ⁴⁺ , U ⁴⁺ , U ⁶⁺ ; Eh-pH conditions; volume fractions of metals/glass and combustibles; initial waste saturation.

Table 3-3. Event-and-Process and Probability-Model Parameters of Consequence Models Used in 1991 WIPP PA Exercises (adopted from Table 6.0-3 of WIPP PA Division, 1991b).

Event-and-Process Parameters:
1. Intrusion borehole diameter
2. Intrusion borehole permeability
3. Recharge amplitude factor under climate change
4. Area of pressurized brine reservoir underlying WIPP site
Probability-Model Parameter:
5. Rate constant in Poisson Drilling Model

probability distribution is really an exercise in mathematical modeling and the product of that exercise may be validly called a *probability model*.

In the present and following sections, the random variable associated with an uncertain parameter, say x , will be denoted by its counterpart expressed in capital letters, say X . A probability distribution for a scalar random variable X can be defined as a nonnegative, nondecreasing function $F(x)$ defined on the range of the parameter x with the following properties:

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$F(x)$ = probability that X is less than or equal to x ;

$F(x)$ tends to zero as x tends towards its lower limit;

$F(x)$ tends to one (1) as x tends towards its upper limit.

Such a function, called a *cumulative distribution function* (or CDF), measures the probability that the random variable X will lie in an interval $[a,b]$, $b \geq a$, of its range:

$$\text{probability that } \{a \leq X \leq b\} = F(b) - F(a) \geq 0.$$

The CDF for an N -dimensional vector of uncertain parameters, say $\mathbf{X}$, can be expressed in a similar fashion:

$$F(\mathbf{x}) = \text{probability that } \{\mathbf{X} \leq \mathbf{x}\}; \quad (3-4)$$

where $\{\mathbf{X} \leq \mathbf{x}\}$ means that

$$X_1 \leq x_1, X_2 \leq x_2, X_3 \leq x_3, \dots, X_N \leq x_N.$$

Expression 3-4 is called a *joint cumulative distribution function* for the set of random variables (i.e., uncertain parameters) $\mathbf{X}$. If $[a,b]$ denotes an N -dimensional interval in parameter space, D_N , such that

$$a_1 \leq b_1, a_2 \leq b_2, a_3 \leq b_3, \dots, a_N \leq b_N,$$

then

$$\text{probability that } \{\mathbf{X} \in [a,b]\} = F(\mathbf{b}) - F(\mathbf{a}).$$

As will be seen later, subsets of D_N like the N -dimensional interval $[a,b]$ can be construed as quantitative representations of *scenarios* (Section 3.3.2).

The function $F(\mathbf{x})$ displayed in Expression 3-4 is intended to be a general expression of a probability model for uncertain parameters appearing in a total-system consequence model (Expression 3-1); the function need not be continuous in all elements of the parameter set, and its arguments, the uncertain parameters, could be partially correlated with one another. Correlations among a model's uncertain parameters may arise from the fact that there are natural correlations between measured quantities that determine their form (e.g., the local values of porosity and permeability of a real rock formation could be empirically correlated); or correlations of uncertain parameters may be implicit in the idealizations made in constructing the mathematical models in which they are used (e.g., local values of fracture porosity are automatically correlated with fracture permeability in some models of fluid flow through fractured rock).

Detecting natural correlations between measured quantities is usually difficult, particularly for measured quantities in the earth sciences, and it is often computationally inconvenient to incorporate known model-derived correlations among uncertain parameters of numerical models of the total system. Consequently, after eliminating those parameters that are known to be functionally dependent upon other problem variables, a model maker might simply assume that the remaining uncertain parameters of a total-system model are statistically independent (see, for instance, WIPP PA Division, 1991b, p. 1-12). This assumption permits the probability model for the total system to be expressed, in an approximate but computationally convenient form, as the product of the marginal distributions of the joint CDF (expression 3-4):

$$F(\mathbf{x}) = F_1(x_1) \cdot F_2(x_2) \cdot F_3(x_3) \cdot \dots \cdot F_N(x_N), \quad (3-5)$$

where N is now the number of uncertain parameters and the $F_n(\cdot)$, $n = 1, 2, 3, \dots, N$, are respectively the CDFs of the individual parameters, x_n , $n = 1, 2, 3, \dots, N$. The form expressed in Equation 3-5 is computationally convenient when certain efficient sampling methods (e.g., the Latin Hypercube Sampling method) are used to implement a stochastic simulation. Techniques for constructing CDFs of individual members of the parameter set are next briefly discussed.

Techniques for constructing CDFs for uncertain model parameters fall roughly into three classes: (1) direct use of data to construct an *empirical* CDF; (2) finding the analytic distribution that best fits available data (e.g., through use of the Kolmogorov-Smirnov test or the chi-squared test), and (3) Bayesian techniques that combine available data and expert judgment to form prior and posterior CDFs (Martz and Waller, 1982). Class 3 includes purely subjective procedures in which no posterior CDF is formed and assignment of a prior CDF relies entirely upon expert judgment. The amount of subjective judgment required by these techniques increases from class 1 to 3; the “best” technique to be used in a particular situation depends strongly upon the kinds and amounts of empirical data and subjective information that are available concerning the parameter.

Construction of empirical CDFs using available empirical data is appropriate if the parameter is intrinsically discrete (e.g., Figure 3-2) or when there are many data points for an intrinsically continuous quantity and that quantity can be related to the parameter by a deterministic, continuous function. The advantage of this technique lies in the fact that the empirical CDF is an unbiased estimator of the population's true CDF (Blom, 1989, p. 121); its disadvantages are that the empirical CDF may not capture probabilities of extreme values at the tails of the distribution, and—for continuous parameters and few data points—the empirical CDF may be too coarse to permit a representative, uniform set of sample values of the parameter to be drawn (as is necessary in implementing certain sampling methods in a stochastic simulation; see Section 3.2.4). The latter disadvantage may in part be offset by joining the vertices of the piecewise constant empirical CDF with straight lines (e.g., Figure 3-3), a procedure that is computationally simple and is justified by the Maximum Entropy Principle (Tierney, 1990).

The two standard techniques for testing whether a data set is consistent with a proposed analytic distribution (i.e., normal, lognormal, beta distributions, etc.) are the chi-squared test and the Kolmogorov-Smirnov test. The chi-squared test is best suited for intrinsically discrete quantities, whereas the Kolmogorov-Smirnov test is most appropriate for intrinsically continuous random variables (Morgan et al., 1990, p. 100). The use of either technique is seldom mentioned in published performance assessments, perhaps because of the sparse data sets so characteristic of measured quantities in the earth sciences or because these tests require lengthy calculations with the data before a distribution is chosen. In connection with PA for the WIPP Project, Pfeifle et al. (1992) have used the Kolmogorov-Smirnov test to find analytic distributions that are consistent with their measurements of certain constants (e.g., Figure 3-4) appearing in a mathematical model of salt creep used in the SANCHO code (see Table 3-1).

TRI-6342-1468-0

Figure 3-2. Distribution of historical drill bit diameter (Fig. 4.2-7, WIPP PA Division, 1991b). (Example of an intrinsically continuous parameter treated as a discrete quantity.)

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TRI-6342-1232-0

Figure 3-3. Measured distribution (pdf and cdf) for tortuosity of Culebra matrix (Fig. 2.6-15, WIPP PA Division, 1991b). (Example of an intrinsically continuous parameter.)

TRI-6342-3719-0

Figure 3-4. Typical comparison between predicted and experimental CDF for the parameter, $\dot{\epsilon}_s$, at $T = 300K$ and $\Delta\sigma = 10 MPa$ (from Pfeifle et al., 1992). (Example of use of Kolmogorov-Smirnov Test to fit a distribution.)

PA analysts in both WIPP and INEL programs have been compelled to adopt techniques from class 3 (Bayesian techniques; also see Section 3.2.2) to construct distributions for most of the uncertain parameters appearing in their consequence models (WIPP PA Division, 1991b). Because of the expense and time required to make and interpret measurements of earth-science quantities or poorly characterized waste-form quantities, the process of constructing CDFs for consequence model parameters has largely bypassed the classical techniques of Bayesian estimation (Martz and Waller, 1982) and has instead relied heavily on subjective judgments of scientific specialists. The elicitation of the judgment of specialists can be either an informal process involving only a few responsible investigators (Figure

3-5), or a formal process involving many experts and rigid controls (Bonano et al., 1990). Examples of distributions obtained by informal and formal elicitations are shown respectively in Figures 3-6 and 3-7.

3.2.4 Stochastic Simulation

Stochastic simulation is a class of computational methods that have been used to explore quantitative uncertainty in a model system's output variables, given measures of uncertainty in the model's input variables; in simple terms, stochastic simulation is a tool for the propagation of parametric uncertainty through complex mathematical models. The distinguishing characteristic of stochastic simulation is the opportunistic exploitation of the mathematical equivalence of *taking the mean value of a set of numbers independently sampled from some distribution and calculating the expected value of a function of a random variable (RV) by direct integration with respect to the RV's underlying probability density function*. Those computational methods that emphasize drawing independent samples of the RV are called *Monte Carlo* methods (Hammersley and Handscomb, 1964; Ripley, 1987); the methods emphasizing direct integration have no special name but are centered around techniques of analytical or numerical evaluation of integrals. Most successful applications of stochastic simulation involve a mixture of the two points of view.

A stochastic simulation requires knowledge of the three objects described in the foregoing three sections of this overview: If uncertain system parameters are regarded as a vector-valued random variable $\mathbf{X}$ defined on the parameter space D_N (Section 3.2.2) and are distributed according to a total-system probability model $F(\mathbf{x})$ (Section 3.2.3), then stochastic simulation with the total-system consequence model $f(\cdot)$ (Section 3.2.1) can give useful estimates of the statistical properties of model consequences, $\mathbf{c} = f(\mathbf{x})$, or any *system performance measure* expressible as a function of model consequences, say $g(\mathbf{c})$.

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Figure 3-5. An informal five-step procedure used to construct cumulative distribution functions (CDFs) for the 1990 WIPP performance simulations (Fig. E-1, Tierney, 1990). (See also Sandia WIPP Project, 1992, for example of formal procedure adopted for WIPP Project.)

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Figure 3-6. Constructed distribution for gas production rates from corrosion under inundated conditions (Fig. 3.3-11, WIPP PA Division, 1991b). (Distribution obtained from informal elicitation.)

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Figure 3-7. Constructed distribution for solubility of plutonium (Fig. 3.3-3(e), Sandia WIPP Project, 1992; see also Figure 9-1, this report). (Distribution obtained from formal elicitation.)

Note on System Performance Measures: Since model "consequences" have so far been given no special meaning in terms of particular types of quantities, there is no loss in generality in assuming that c [instead of $g(c)$] represents whatever numerical measures of system performance are to be explored by the user of the model. Thus, in the remainder of this overview, c [or $f(x)$] will mean either a vector of consequences or a vector whose elements are system performance measures. If there is only one performance measure, then that measure will be denoted by a scalar (not bold) " c ". For example, the performance measure that is to be tested against EPA's standard (see Section 2.3.2) is of the form

$$c = \sum_{i=1}^I \frac{M_i}{L_i}$$

where the sequence of numbers $\{M_i\}$ are model consequences (in this example, the cumulative radioactivity released to the accessible environment in the form of the i th radionuclide during a 10,000-yr period); the numbers $\{L_i\}$ are normalization factors defined by the EPA; and I is the number of radionuclides considered in forming releases to the environment.

Uncertainty in a performance measure c can be quantified in several ways: At the very least, estimates of the mean value and variance of the distribution of C are needed to roughly center the distribution and estimate its width. In many applications (e.g., compliance with EPA's standard; see Section 3.1), an estimate of the entire CDF for the performance measure is required. According to the mathematical theory of probability (see Feller, 1966), all moments and distributions of the function of a random variable, $C = f(X)$, may in principle be calculated by taking the expected value of certain functions of C , i.e., by evaluating integrals of the form

$$E[h] = \int_{D_N} h[f(x)] dF(x) \quad (3-6)$$

where the integral is taken over the entire parameter space, D_N , and $dF(x)$ can be interpreted as a generalized derivative of the total-system probability model $F(x)$. (Note: integrals of the kind shown in Expression 3-6 are called Lebesgue-Stieltjes integrals [Feller, 1966]; this generalized theory of integration becomes necessary when $F(x)$ is not differentiable in all of its arguments.) Possible choices for the functions $h(\cdot)$ will be described below along with practical methods of numerically evaluating Lebesgue-Stieltjes integrals over multidimensional spaces.

Expression 3-7 defines the *expectation operator*, $E[\cdot]$, whose operational meaning should be obvious: take an arbitrary but well-behaved function $h(x)$, weight it with the infinitesimal probability $dF(x)$, and integrate the product over all values of $x \in D_N$. The expected (or mean) value of the components of performance measure C can be calculated by taking

$$h(x) = f_i(x), \text{ for each } i = 1, 2, 3, \dots, N.$$

The covariance matrix of the performance measure C is found by taking

$$h(x) = [f_i(x) - E_i(h)][f_j(x) - E_j(h)],$$

$$\text{for all } i, j = 1, 2, 3, \dots, N,$$

where the expressions $E_i(h)$ and $E_j(h)$ stand for the expected (or mean) values of the i th or j th component of f .

The full joint CDF for the performance measure C may be calculated by taking

$$h(x) = \prod_{i=1}^N u[f_i(x) - c_i],$$

where $u(\cdot)$ stands for the unit step function, a function having the properties $u(z) = 1$ if $z \geq 0$ and $u(z) = 0$ if $z < 0$. In this case, application of the expectation operator to $h(x)$ gives $G(c)$, the probability that

$$C_1 \leq c_1, C_2 \leq c_2, C_3 \leq c_3, \dots, C_N \leq c_N,$$

where $c_1, c_2, c_3, \dots, c_N$ are now independent variables; i.e., they can take arbitrary values within their natural ranges. As a last example of the expectation-operator formalism, the full expression for the CDF of a scalar performance measure C is displayed below.

$$G(c) = \int_{D_N} u[c - f(x)] dF(x) \quad (3-7)$$

In the context of the EPA standard, if $f(x)$ is the normalized cumulative release of radioactivity in a 10,000-yr period following closure of a waste-disposal site that is predicted by the total-consequence model when given a parameter set x , then the "overall probability distribution" called for by the Standard is precisely the *complementary cumulative distribution function* (CCDF), $1 - G(c)$, with $0 \leq c < \infty$.

Practical Stochastic Simulation. In stochastic simulation, the problem of computing the multi-dimensional integrals of Expression 3-7 is second in importance only to the problems of creating realistic and computationally efficient consequence and probability models. It is seldom possible to evaluate all integrals appearing in Expression 3-7 by analytical means or by direct numerical integration: the dimension of integration is usually large, possibly involving tens or hundreds of parameters, and one or both of the integrands, $h[f(x)]$ and $dF(x)$, may be communicable only in terms of complex numerical algorithms or computer code. Monte Carlo methods are perhaps the only universally applicable techniques for evaluating these multi-dimensional integrals. The following is a brief outline of the simplest of the Monte Carlo methods, the "random-sampling" method.

To calculate an estimate of $E[h]$ (Expression 3-7) with the random-sampling method, one begins by drawing $M \gg 1$ sample values of the parameter-set vector, say $X_1, X_2, X_3, \dots, X_M$, from the total-system probability model $F(x)$. (Chapter 11 of Ross [1985] is a good introduction to techniques for "drawing" independent samples of a random variable from its associated CDF.) Next, one computes the quantities $h[f(X_m)]$, $1 \leq m \leq M$, and forms their arithmetic mean:

$$\langle h \rangle = \frac{1}{M} \sum_{m=1}^M h[f(X_m)] \quad (3-8)$$

The quantity $\langle h \rangle$ is called an *estimator* of the expected value of $h[f(x)]$; by the equivalence mentioned earlier, it is also an estimate of the integral shown in Expression 3-7. Depending upon the size of the sample, M , there will be an error (i.e., the difference between the exact value of Expression 3-6 and the estimated value given by Expression 3-9) associated with this procedure. Brief discussions of the error term can be found in Ross (1985) and in Tierney (1991, p. 3-11); in general, the error associated with the random-sampling method is inversely proportional to the square root of the sample size M .

Note again that by an appropriate choice of the function $h[\cdot]$ in Expression 3-9, one may calculate estimators of mean value, variance, and of the CDF of the performance measure C . In particular, the estimator of the CCDF of the EPA's performance measure (expression 3-9) takes the form

$$\langle 1 - G(c) \rangle = \frac{1}{M} \sum_{m=1}^M u[f(X_m) - c] \quad (3-9)$$

This estimator takes the form of an empirical CCDF (see Section 3.2.3), i.e., the sum of M unit step functions, and has the appearance of a series of descending stair steps (Figure 3-8). As the sample size M becomes large, the empirical CCDF will approach the smooth curve representing the true CCDF for the population of performance measures that is implicit in the total-system model under consideration.

The major drawback associated with the random-sampling method is that a large number of samples of the parameter-set vector must be taken to keep the sampling error within acceptable bounds. Random sampling may be impracticable when used with consequence models implemented by large and complex computer codes that require substantial time and storage to complete a calculation of a single sample consequence. In these situations, computer-

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Figure 3-8. An example of an empirical CCDF (modified from Fig. 3.6 in Rechard, 1989).

time requirements may be reduced by employing other variants of Monte Carlo methods such as stratified sampling (Kalos and Whitlock, 1986) or the related Latin hypercube sampling (LHS) (Iman and Conover, 1982); use of these variant methods will, for the same sample size M , often reduce variance of the estimates of the performance measures below the variance dictated by the random-sampling method. Unfortunately, making a priori estimates of the error associated with use of the LHS estimator in a non-linear model is difficult, and one usually has to estimate the sampling error after the fact of the calculation. Iman and Helton (1985, p. 2-5) have conducted numerical experiments with LHS on a variety of models; their experience shows that tolerable levels of sampling error are achieved when M is chosen to be greater than $(4/3)N$, where N is the number of uncertain parameters to be sampled.

An Example from the WIPP PA. The WIPP PA Department at Sandia National Laboratories and INEL project analysts have employed a combination of LHS and direct integration in their preliminary calculations of conditional CCDFs for the normalized cumulative release of radioactivity from geologic repositories (this is the performance measure expressed above in Equation 3-9). A full description of the theoretical approach to these calculations is given in Helton (1993) and the particular computational approximations used in these calculations are described in Chapter 3 of WIPP PA Division (1991a); typical results from these simulation exercises are shown on Figure 3-9. A technical but brief discussion of the WIPP PA Department's approach to stochastic simulation is also supplied in the last section (3.3) of this overview.

The reader will notice that Figure 3-9 displays a *family* of CCDFs. Each curve in this family is the result of a conditional simulation in which integration is performed (approximately and numerically in this example) over a small subset of the uncertain parameters, while the remainder of elements of the parameter-set vector are held fixed at values chosen by the LHS sampling scheme. Thus there is one conditional CCDF for each of the LHS sample vectors, say $\mathbf{X}_m$, $m = 1, 2, 3, \dots, M$. These M curves may be combined and analyzed with the methods of ordinary statistics: the arithmetic average of the M curves is an estimator of the true CCDF for the population of performance measures implicit in the PA analyst's consequence and probability models; and various "percentile" CCDFs may be formed by simple numerical interpolation of the M curves (Figure 3-10, taken from Helton, 1993).

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Figure 3-9. Example family of CCDFs generated by Latin hypercube sampling for comparison with the EPA release limits (Fig. 13 in Helton, 1993).

Figure 3-10. Mean and percentile curves for the family of CCDFs shown in Figure 3-9 (Fig. 14 in Helton, 1993).

Caveats for Interpretations of Figures 3-9 and 3-10. The reader may also have noticed that one member of the family of CCDFs displayed in Figure 3-9 exceeds the limits of the Containment Requirements. This observation may lead to the conclusion that the geologic repository being studied, at least as it is presently being modeled, is not likely to comply with the Containment Requirements of 40 CFR 191 (see Chapter 2). In reply to such a conclusion, we can only remark that *one should be cautious about making regulatory interpretations of conditional CCDFs such as those displayed in Figure 3-9*. There are at least two good reasons for exercising caution: First, conditional distributions (CDFs or CCDFs) are themselves chance quantities (or random variables) to which probabilities should be attached before any interpretations of their significance are made. Realizations of conditional distributions, such as those displayed in Figure 3-9, can be viewed as "samples" independently drawn from an unknown "distribution of distributions" whose structure can be investigated using standard techniques of statistics; one instance of the use of standard techniques is the plotting of various percentiles and the calculation of a mean curve as shown in Figure 3-10. Another way of analyzing the significance of the set of curves in Figure 3-9 would use repeated sampling to estimate the frequency that the sample curves exceed the limits of the Containment Requirements; for the sample shown in Figure 3-9, the estimated frequency of exceeding the limits is obviously 1/40 (0.025).

Second, and most important, a conditional distribution of the kind whose samples or realizations are exemplified in Figure 3-9 cannot be a unique and statistically stable measure of performance for the total-system model. To see why this is so, recall that conditional distributions are obtained by holding fixed certain members of the set of uncertain parameters while computing the expectation of the performance measure (Eq. 3-6) with respect to the remaining members of the uncertain-parameters set. *The choice of the parameters to be held fixed in computing conditional distributions is arbitrary and usually depends upon the purposes of the analysis.* In the example of Figure 3-9, the expectation integral was analytically taken over the small set of parameters that specified the number of inadvertent intrusions into the WIPP site during five 2000-yr time intervals; the remaining uncertain parameters, called "subjectively uncertain" parameters by Helton (1993, p. 37), were consecutively assigned the 40 vector values sampled by the LHS scheme. This choice of the set of fixed parameters and the set of parameters over which the expectation integral was taken was dictated only by considerations of computational economy and convenience; other considerations might have dictated a different choice that would lead to a family of realizations that differ considerably from those shown in Figure 3-9.

The cautions offered above may suggest an answer to a question that frequently arises in connection with families of empirical CCDFs such as those exemplified in Figure 3-9 and statistically ordered or averaged in Figure 3-10: Which curve should be used to assess compliance with the Containment Requirements? The mean curve, the median curve, or the 90th percentile? We believe the answer is the mean curve, for the mean curve is the result of taking the expectation of the performance measure with respect to all uncertain parameters and is therefore independent of arbitrary choices of the conditioning parameters (it is also an unbiased estimator of the unknown, underlying CCDF for the model system). Of course, uncertainty in the estimated mean curve must be quantified, but this can be done using standard statistical techniques as indicated above.

3.3 Scenarios and Conditional Simulation

This section is a treatment of several topics of special interest to performance assessment of geologic waste-disposal systems. The many definitions of "scenario" are sampled and briefly discussed in Sections 3.3.1 and 3.3.2 and a practically usable definition of "scenario" is proposed in the latter section. Section 3.3.3 is a development of the idea of expanding a performance assessment in a series of "scenarios", an idea which is shown to be equivalent to expansion in a series of conditional simulations. Section 3.3.4 is a reconciliation of the formalism of stochastic simulation presented in Section 3.2 with the Kaplan-Garrick representation of risk (Kaplan and Garrick, 1981) that forms the basis of performance assessments of the WIPP and INEL systems.

3.3.1 Definitions of 'Scenario'

The wide range of meaning attached by PA workers to the noun "scenario" has rendered the word nearly useless for the purpose of technical communication. Six different definitions of "scenario" are mentioned below; even among these few definitions there are instances in which the authors' intentions are not entirely clear.

1. *Scenario selection* and *scenario screening* name two steps in the mainly heuristic act of identifying important events, processes and features that can cause or influence significant releases of radioactivity to the accessible environment from a waste-disposal system (Cranwell et al., 1990; Hunter, 1989; Guzowski, 1990).
2. A *summary scenario* (WIPP PA Division, 1991a, p. 1-3) is a member of the class of all subsets (including the "empty" set) of the set of all distinct disruptive events, uncertain features, and alternative conceptual models that were identified by scenario selection and screening (Tierney, 1991, pp. 3-22 to 3-26). The empty set is often called the *base-case scenario* in PA work.
3. A scenario is "a set of similar occurrences" (Helton, 1993, p. 26), i.e., a set of things that can happen and, if they happen, have in some sense similar outcomes or consequences.
4. A *computational scenario* (WIPP PA Division, 1991a, p. 2-7) is a member of a class of subsets of parameter space obtained by dividing the parameter space of a summary scenario into units that are computationally convenient for partial evaluation of expectation integrals of the kind typified in Equation 3-6.
5. A scenario is a point in parameter space; $x \in D_N$ (Morgan et al., 1990, p. 174; Tierney, 1991).
6. A *scenario class* is a subset of parameter space (Tierney, 1991, Appendix A).

Regarding definition 1: In Chapter 7, Scenario Development, the terms *scenario selection* and *scenario screening* are used as synonyms for two necessary steps in the construction of any model of a natural or engineered system: (1) deciding upon the physical, chemical and anthropogenic phenomena that *might* play a significant role in determining the performance of the system; and (2) deciding upon which of the phenomena identified in Step 1 *must* be incorporated in a mathematical model of the system if that model is to predict all consequences of interest to investigators. It appears that Steps 1 and 2 correspond to the steps of "translation from real-world data" and "induction from experience" that are at the heart of the cyclical process of mathematical modeling (Figure 3-11). The scenario-selection methodology proposed by Cranwell et al. (1990) is no more than a set of guidelines that a PA analyst may profitably follow in making the necessary inductions and translations from real-world data and experiences.

Regarding definition 3: Helton's intentions in posing this definition of scenario (Helton, 1993, p. 26) are not entirely clear, but from the context in which the word is used in his paper, one may infer that he is trying to connect certain computational scenarios (definition 4) with the first member of Kaplan and Garrick's representation of risk as a triplet: $\langle s_i, p_i, x_i \rangle$, where " s_i is a scenario identification or description; p_i is the probability of that scenario; and x_i is the consequence or evaluation measure of that scenario, i.e., the measure of damage" (Kaplan and Garrick, 1981, p. 13). An interpretation of the Kaplan-Garrick triplet in terms of subsets of, and probability measures on, the total-system parameter space is supplied in Section 3.3.4.

The reader may convince herself that the remaining definitions of "scenario"—2, 4, 5, and 6—have a practical meaning only after a mathematical model has been constructed and the analyst is ready to make numerical predictions with the model (the "prediction-deduction" step in Figure 3-11). At this point in the modeling cycle, a (perhaps preliminary) total-system consequence model (Section 3.2.1) and its associated parameter space (Section 3.2.2) exist and their concrete features can be displayed, examined and analyzed. The need for precise communication of model features dictates that, if used at all, the word "scenario" should at this point denote some common property of those features that is also useful as an analytical or computational tool. Since definitions 5 and 6 are already clear definitions in the sense of denoting concrete model features, only definitions 2 and 4 require further discussion and analysis. In the next section, it is proposed that the terms *summary scenario* and *computational scenario* be used to denote certain subsets of the model's parameter space.

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Figure 3-11. The cyclical nature of mathematical modeling (Roberts, 1976; Figure 1-1).

3.3.2 Scenarios as Subsets of Parameter Space

The dictionary definition of “scenario” judged to be nearest to PA analysts’ definitions is “an outline of a hypothetical chain of events” (American Heritage, 1975). Note that such an outline of events could take precise and economic narrative form as a series of simple statements—e.g., “Xavier is blue., Mary is less than three., John is ill.”—linked by the conjunction “and”. In each simple statement, a subject (e.g., Xavier, Mary, John) is assigned a quality or property (e.g., respectively, blue, less than three, ill). Note also that a family of outlines of events can be generated by allowing one or more of the qualities/properties appearing in the simple statements to be free variables, e.g.,

“Xavier is m ”, where m is degree of pleasure;

“Mary is less than a ”, where a is age in years;

“John is h ”, where h is degree of health.

Simplistic reflections of this kind concerning the commonly accepted definition of scenario lead to the idea of defining the “scenarios” of performance assessment in a similar but slightly stronger way:

In PA work, a *scenario* is a compound statement, $A(\mathbf{x})$, that is built by linking with the conjunction “and” any series of simple statements about values taken by elements of the parameter vector, $\mathbf{x}$, and/or the vector of consequences, $\mathbf{f}(\mathbf{x})$.

It is easily seen that this definition establishes a correspondence between properly phrased, qualitative statements about the behavior of the *model system* and certain sets of points in the parameter space D_N . For any given scenario $A(\mathbf{x})$, there is a (possibly empty) subset of D_N defined by

$$S = \{\mathbf{x}: \mathbf{x} \in D_N \text{ and } A(\mathbf{x}) \text{ is true}\}.$$

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The expression above reads as follows: "S is the set of all x contained in the parameter space for which the statement $A(x)$ is true". The complement of S,

$$S^c = \{x: x \in D_N \text{ and } A(x) \text{ is false}\},$$

is also a subset of D_N ; it corresponds to the statement,

$$A'(x) = \text{the negation of } A(x).$$

Thus, subsets of parameter space defined in this way, i.e., by the truth value of a statement, may also be called "scenarios" without confusion.

In addition to establishing an operationally useful association between most qualitative assertions about the behavior of the system (i.e., "scenarios" in the sense of Hunter, 1989 and Guzowski, 1990) and subsets of the parameter space, this definition of scenario solves the long-standing problem of assigning probabilities to scenarios: The probability of a scenario, $A(x)$, is simply the probability of its associated subset S, a quantity that can be calculated by means of the total system's probability model (Section 3.2.3). A discussion of methods for calculating scenario probabilities is deferred to Section 3.3.3. At this point, it is appropriate to give some examples of different kinds of scenarios and their associated subsets. The first example is a simple but general one that demonstrates some of the advantages to be gained by defining scenarios in terms of subsets of the parameter space.

Example 1. *Envelope of acceptable system performance.* Suppose that $f(x)$ is a scalar performance measure for a total system and that the performance of the system is judged to be acceptable if that performance measure falls within a prescribed interval (a,b) of the real line. The scenario of acceptable system performance, expressed as a subset of parameter space, is obviously

$$S(\text{acceptable}) = \{x: x \in D_N, a < f(x) < b\}.$$

Normally, the system's analysts are not interested in the scenario of acceptable performance per se, but in the *likelihood* that the particular system (here specified by the function $f[\cdot]$) will perform acceptably. As shown in the following section, the likelihood (probability) that the system performs acceptably is identical to the probability measure attached to the set $S(\text{acceptable})$; the latter can be estimated (perhaps at considerable computational expense) by a Monte Carlo simulation with the total system model that calculates $f(x)$ and the total-system probability model (Section 3.2.3) that calculates the joint CDF, $F(x)$, for the vector of uncertain parameters x .

Example 2. *Summary Scenarios* as subsets of parameter space can be exemplified using a hypothetical situation in which R1 and R2 designate two different kinds of chance events that could disturb the operation of the waste-disposal system (e.g., exploratory drilling, earthquakes), and T1, T2, T3 designate three different kinds of uncertain features of the waste-disposal system (e.g., an undetected fault zone, an undetected brine pocket, and an undetected universal flaw in waste containers). Suppose that these five agents are the only significant chance events and uncertain features that were identified during the qualitative scenario screening process and that mathematical submodels of the effects of each agent upon system performance measures have been constructed and included in the total-system consequence model. It is also assumed that certain processes (e.g., groundwater flow) are operating everywhere and at all times, though at imprecisely known levels.

The five agents may be listed as elements of a set, viz., $\{R1, R2, T1, T2, T3\}$, whose subsets, e.g., $\{R2, T3\}$, $\{R1\}$, etc., have the following meaning: the elements that appear in a subset occur at least once (in the case of an event) or are present (in the case of a feature) during the period of performance of the waste-disposal system. Since none of the five disturbing agents necessarily occurs or is necessarily present during the period of performance, an "empty" subset—here denoted simply by $\{\}$ —must be introduced to allow for the *base case* of "undisturbed" or "nominal" performance. The set $\{R1, R2, T1, T2, T3\}$ has exactly 32 subsets including the empty subset (i.e., 2^N subsets, where $N = 5$ in this example); these subsets can be enumerated and classified by means of a logic diagram (Figure 3-12). The 31 subsets plus the base case are called "summary scenarios" in WIPP PA practice (WIPP PA Division, 1991a).

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Figure 3-12. Logic diagram for the construction of summary scenarios (adapted from Guzowski, 1990).

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A practical meaning may be associated with each summary scenario by a statement expressing the presence or absence of each event or feature in the subset: for example, the subset {R1,T2,T3} can be interpreted by the statement

“R1 occurs at least once during the period of performance
and
T2 is present
and
T3 is present
and
R2 does not occur and T1 is not present.”

It is next shown that such compound statements place unique numerical constraints on uncertain parameters of the total system: If N1, N2 are parameters representing respectively the number of times events R1, R2 occur in the period of performance and I1, I2, I3 are binary parameters representing respectively the presence (I = 1) or absence (I = 0) of features T1, T2, T3, then the statement above can be recast in the symbolic form

$$B(x) = (N1 > 0, N2 = 0, I1 = 0, I2 = 1, I3 = 1)$$

where it is understood that all elements of the vector x but elements (N1,N2,I1,I2,I3) can take arbitrary values within their allowable ranges. The set defined by

$$S = \{x: x \in D_N \text{ and } B(x) \text{ is true}\}$$

is a unique subset of the parameter space D_N . Furthermore, this set is but one of 32 subsets of D_N that can be built from the 32 summary scenarios (Figure 3-12) using the procedure described above (i.e., translation of presence or absence of a feature or event into a statement about problem parameters). The reader may convince himself that these 32 subsets exhaust the parameter space in the sense that their union equals D_N ; furthermore, the 32 subsets are mutually disjoint in the sense that no two of them share a common element x. As will be seen in the next section (3.3.3), the fact that members of the class of subsets representing the class of summary scenarios are both exhaustive and mutually disjoint permits a convenient expansion of a PA calculation for a CCDF into a series of conditional simulations each involving a summary scenario.

Example 3. A *computational scenario* is a member of a class of subsets of parameter space that is obtained by subdividing the subspace S spanned by parameters of a summary scenario (Figures 3-12 and 3-13). As an object on which to focus this example, consider the summary scenario {R1, T2, T3} discussed in Example 2: the statement defining this summary scenario was expressed in symbolic form as

$$B(x) = (N1 > 0, N2 = 0, I1 = 0, I2 = 1, I3 = 1),$$

where N1 counts the number of times the event R1 occurs during the period of performance (see Example 2 for definitions of the other parameters). As argued in Example 2, the summary scenario B(x) corresponds to a unique set of points in parameter space,

$$S = \{x: x \in D_N \text{ and } B(x) \text{ is true}\}.$$

Notice that B(x) is true for all x in which the parameter N1 takes integer values greater than zero.

Now suppose that, for convenience in numerical calculations, an investigator needs to distinguish the occurrences of the chance event R1 in each of five, disjoint time intervals dividing the period of performance: To make this distinction, he might begin by creating a vector of random variables, $N = (N_1, N_2, N_3, N_4, N_5)$, in which the N_i , $1 \leq i \leq 5$, stand for the number of times event R1 occurs during the *i*th interval of time; the constraints imposed by the choice of summary scenario on N are only that

$$N1 = N_1 + N_2 + N_3 + N_4 + N_5$$

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Figure 3-13. Schematic illustrating partitioning of parameter space into summary scenarios and computational scenarios.

be an integer greater than zero. The hypothetical investigator might next define a family of scenarios by the statement (given here in symbolic form),

$$C(\mathbf{x}, \mathbf{n}) = (N_1 = n_1, N_2 = n_2, N_3 = n_3, N_4 = n_4, N_5 = n_5),$$

where $\mathbf{n} = (n_1, n_2, n_3, n_4, n_5)$ is vector of non-negative integers not all of which are zero. The family of scenarios induced by this statement corresponds to a family of sets,

$$S(\mathbf{n}) = \{\mathbf{x}: \mathbf{x} \in D_N \text{ and } [B(\mathbf{x}) \text{ and } C(\mathbf{x}, \mathbf{n})] \text{ is true}\},$$

that composes an exhaustive, mutually exclusive partition of the summary scenario's parameter space. Members of a family of sets constructed in this way have been given the name *computational scenarios* (WIPP PA Division, 1991a).

3.3.3 Probability of a Scenario, Conditional Simulation

The idea of an *indicator function* of a set S will be helpful in explaining scenario probabilities and conditional simulation. If S is a subset of D_N , then the indicator function of S is the function defined on D_N with the properties,

$$I(S, \mathbf{x}) = 1 \text{ if } \mathbf{x} \in S,$$

$$I(S, \mathbf{x}) = 0 \text{ if } \mathbf{x} \notin S.$$

If the set S is a scenario in the sense of Section 3.3.2 (i.e., a subset of D_N defined by a statement $A(\mathbf{x})$) then, since $\mathbf{x} \in S$ if and only if $A(\mathbf{x})$ is true, one can also define its indicator function by

$$I(S, \mathbf{x}) = 1 \text{ if } A(\mathbf{x}) \text{ is true,}$$

$$I(S, \mathbf{x}) = 0 \text{ if } A(\mathbf{x}) \text{ is false.}$$

The latter definition of indicator function is useful for numerical calculations: Given a sample parameter vector $\mathbf{X}$, the value for $I(S, \mathbf{X})$ can be calculated simply by testing whether $A(\mathbf{X})$ is true or false.

Probability of a Scenario. A meaning can now be given to *probability of a scenario*. The probability of a scenario, $P(S)$, is the expectation of the scenario's indicator function, i.e.,

$$P(S) = \int_{D_N} I(S, \mathbf{x}) dF(\mathbf{x}).$$

A Monte Carlo estimator for $P(S)$ will therefore look like

$$\langle P(S) \rangle = \frac{1}{M} \sum_{m=1}^M I(S, \mathbf{X}_m).$$

(see Eq. 3-9), where the $\mathbf{X}_m$, $m = 1, 2, 3, \dots, M$, are independent samples of the parameter vector obtained by random sampling or LHS.

The Monte Carlo estimator for $P(S)$ clearly expresses the frequentist's definition of probability: Draw M independent sample variates and count the number of samples that satisfy some criteria (i.e., are "successful" trials); the ratio of the number of successes to the total number of trials gives an estimate of the probability that the criteria are satisfied. In spite of its simplicity, Monte Carlo estimation of scenario probabilities is rare in PA practice, perhaps because of the expense involved in evaluating the truth of $A(\mathbf{x})$ whenever that statement places conditions on an expensive-to-calculate performance measure $f(\mathbf{x})$; in fact, the only instance of a Monte Carlo estimation of scenario probability of which we are aware is the calculation of the CCDF for the EPA performance measure (see Eq. 3-10). If the statement defining the scenario places no conditions on performance measures, it should be quite easy to estimate scenario probabilities by Monte Carlo simulation; admittedly, in such a case it may be even more efficient to calculate those probabilities using logic diagrams (Figure 3-12) and probability models of the agents (events, features, process representations) that are included in the underlying summary scenario.

Conditional Simulations. It has proven useful and revealing in PA work to study system performance by restricting the model system's configurations to those allowed by a particular summary scenario; in other words, the total-system model's "universe" is narrowed to the sum of all things that could happen in the more restricted universe of a summary scenario. Some (Helton, 1993) call this technique "importance sampling," because the summary scenario chosen for special attention is usually the one investigators believe will contain the most unfavorable, hence important, consequences. In the context of stochastic simulation, importance sampling is a subcase of a technique usually called *conditional simulation*.

All of the formulae of Section 3.2.4 that applied to stochastic simulation of the total system will, with some simple modifications, also apply to a conditional simulation with respect to a scenario S . Assuming that $P(S) > 0$, the *conditional expectation* of a performance measure, $h[f(\mathbf{x})]$, with respect to a scenario S can be defined:

$$\mathbb{E}[h/S] = \frac{1}{P(S)} \int_{D_N} I(S, \mathbf{x}) h[f(\mathbf{x})] dF(\mathbf{x}).$$

The left side of the above expression is to be read as "the conditional expectation of $h[f(\mathbf{x})]$ given the scenario S ". Note the similarities and differences between this expression and Equation 3-6. As an exercise, the reader should try

to form the expression for the Monte Carlo estimator of the conditional expectation of a performance measure $h[f(\mathbf{x})]$ (see Eq. 3-9).

A technique frequently used in PA work is the expansion of a total-system performance measure in a series of performance measures of "scenarios", i.e., a series of conditional simulations, each of which is constrained to a given member of a set of summary scenarios. Let the parameter space D_N be partitioned into L summary scenarios, $S_1, S_2, S_3, \dots, S_L$, which obey the following conditions:

$$S_l \cap S_m = \phi, l \neq m; \quad \bigcup_{l=1}^L S_l = D_N$$

and suppose that all the $P(S_l)$ are > 0 . Then, because of the second of the two conditions above,

$$I(D_N, \mathbf{x}) = \sum_{l=1}^L I(S_l, \mathbf{x}) = 1 \quad \text{for all } \mathbf{x} \in D_N$$

and it follows that

$$\mathcal{E}[h] = \sum_{l=1}^L \int_{D_N} I(S_l, \mathbf{x}) h[f(\mathbf{x})] dF(\mathbf{x}) = \sum_{l=1}^L P(S_l) \mathcal{E}[h | S_l].$$

For example: If $f(\mathbf{x})$ is the performance measure for the EPA standard and $h[f(\mathbf{x})] = u[f(\mathbf{x}) - c]$, (see Eq. 3-8 and following text), then $\mathcal{E}[h]$ is the CCDF for the normalized cumulative release of radioactivity in a 10,000-yr period following closure and the $\mathcal{E}[h | S_l]$ are CCDFs for normalized cumulative release that are conditioned upon the realization of only those events and features included in the l th summary scenario; note that in forming the sum over all summary scenarios, each conditional CCDF is weighted by the probability of its summary scenario.

3.3.4 Construction of CCDFs in the WIPP PA

A formalism developed by Kaplan and Garrick (1981) is extensively used in WIPP and INEL PA work to justify certain approximate methods for the calculation of conditional CCDFs (WIPP PA Division, 1991a). This section reconciles the Kaplan-Garrick formalism with the theory of stochastic simulation presented in Sections 3.2.4 and 3.3.3. In Helton's notation (Helton, 1993), the Kaplan-Garrick risk triplet is defined as follows:

$$R = \{(E_i, pE_i, cE_i), i = 1, 2, 3, \dots, nE\}$$

where

- E_i = a set of similar occurrences
- pE_i = probability that an occurrence in set E_i will take place
- cE_i = a vector of consequences associated with E_i
- nE = number of sets selected for consideration.

The correct correspondence between the formulae of this overview (e.g., see Eq. 3-10) and the risk-triplet formalism is made by letting $S_l \leftrightarrow E_i$, $P(S_l) \leftrightarrow pE_i$, $L \leftrightarrow nE$ and, for a vector performance measure of the form $h[f(\mathbf{x})] = f(\mathbf{x})$ (i.e., where the performance measure is consequences),

$$\mathcal{E}[h | S_l] \leftrightarrow cE_i.$$

3. PA Methodology Overview

Helton (1993, p. 19) shows how to construct an empirical CCDF for a scalar consequence value cE using the Kaplan-Garrick formalism; this is done by plotting the points,

$$\left(cE_i, \sum_{j=i}^{nE} pE_j \right) \quad i = 1, 2, 3, \dots, nE$$

to form the usual "descending stair steps" histogram.

4. Description of Waste and Waste Parcels

J. S. Rath and R. P. Rechar

This section describes the types of spent fuel and waste being studied in the 1994 PA, including the waste types, their volume and mass, radionuclide inventory, treatment options, and containers. For the purposes of this performance assessment, waste refers to the contents of a nuclear waste container (with the exception of internal backfill) and comprises components such as fuel rods, brackets, hardware, and modified high-level waste.

4.1 Description of Waste Types

Both spent nuclear fuel and high-level waste are being considered in the 1994 PA. Five types of spent nuclear fuel are included in this performance assessment: four from INEL and one from Hanford. All waste types from INEL primarily originate with spent fuel that has been accepted for interim storage and reprocessing since 1953 by DOE at the Chem Plant. There are over 90 types of fuels being stored at INEL, most of them at the Chem Plant. These 90 types of spent nuclear fuels are categorized for this study as graphite spent fuel, highly enriched uranium (HEU) spent fuel (represented by advanced test reactor [ATR] fuel), robust highly enriched uranium spent fuel (represented by spent fuel from the Shippingport reactor), low enriched uranium (LEU) spent fuel (represented by pressurized water reactor [PWR] commercial fuel), and weapons production spent fuel (represented by N-Reactor fuel spent fuel).

The calcine high-level waste from INEL was produced during reprocessing of spent nuclear fuel at the Chem Plant. The performance assessment also includes high-level waste as borosilicate glass from three DOE sites: Savannah River, Hanford, and West Valley.

Brief descriptions of the waste types are provided below. Additional information can be found in Appendix A.

4.1.1 Description of Graphite Spent Fuel (Fort St. Vrain)

Two kinds of graphite spent fuel are included in the radionuclide inventory: fuel from Fort St. Vrain (Figure 4-1) and Peach Bottom Cores I and II. Both fuels contain a homogeneous mixture of two types of particles, fissile and fertile. As manufactured and prior to irradiation, fissile particles contain thorium and 93.5% enriched uranium; fertile particles contain only thorium. The fuel kernels are coated with three fission-product retaining layers by means of a fluidized-bed vapor-phase deposition process. The inner and outer layers are of isotropic carbon, and the middle layer is of silicon carbide (SiC) (hence the name, TRISO-coated). A fourth layer of porous carbon, called the "buffer," is next to the kernel of fissile or fertile material and provides a volume for accumulation of fission-product gases without excessive pressure buildup. The SiC layer is highly resistant to both oxidation and moisture, even at extremely high temperatures. In the Fort St. Vrain design, the fissile and fertile particles are blended and then molded into 1.27-cm diameter $\times$ 5.08-cm long fuel rods (compacts).

Differences between Fort St. Vrain and Peach Bottom spent fuel are that (a) the Peach Bottom Core 1 particles do not contain the protective SiC layer and (b) the Peach Bottom compacts are 6.86-cm outside diameter, 4.25-cm inside diameter $\times$ 7.57-cm-long hollow cylinders. For the 1994 PA, the graphite fuel is modeled primarily with the characteristics of the fuel from Fort St. Vrain. The results of the 1993 PA indicated that the differences between the two types of fuels were slight in regard to parameters of significance. An exception is that the graphite fuel from Peach Bottom had a significant fraction of fuel particles that failed. Therefore, the 1994 PA uses the distribution for failed particles that includes both the Fort St. Vrain and Peach Bottom graphite fuels (i.e., the distribution for Waste Disposal Group 1, WP 1, from the 1993 PA). A summary of data about the graphite spent nuclear fuel category is provided in Table 4-1.

4. Description of Waste and Waste Parcels

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Figure 4-1. Fort St. Vrain whole block element.

Table 4-1. Data Summary for Graphite Spent Nuclear Fuel *

Description	Units
Volume (as is)	293 m ³
Mass (gross weight)	352 MT 28 MTHM
Thermal Output (year 2030)**	48.5 W/m ³
Radionuclide Inventory (year 2030)	4.23 × 10 ⁶ Ci
Uranium Enrichment	50 - 93%

* See also Appendix A. These values are based on information available at the time of analysis and could change in response to new data.
 ** The thermal output values are calculated from the radionuclide inventory.

4.1.2 Highly Enriched Uranium (HEU) Spent Nuclear Fuel (ATR Fuel)

The highly enriched uranium (HEU) spent fuel category is represented by fuel that originated in the Advanced Test Reactor (ATR), which was designed as an experimental test reactor and provided for the insertion of numerous experiments into the core. The core and fuel were designed to produce a more heterogeneous flux than a pressurized water reactor (PWR). The ATR has four mechanical systems for reactivity control instead of the usual single system.

The ATR fuel is contained in plates of an aluminum-uranium matrix, which is clad with pure aluminum (Figure 4-2). The fuel assemblies contain no control rods or other control components found in most PWR fuel assemblies. Each element forms a 45-degree sector of a right circular cylinder (wedge-shaped) and consists of 19 fuel plates with coolant channels between each plate. The fuel plates are 1.26 m (49.5 in.) long, with an active fuel length of 11.22 m (48 in.) and are loaded with a highly enriched uranium matrix consisting of uranium-aluminide (UAl₃) and clad in ASTM B 209 aluminum alloy 6061-TG. The total fuel content of an ATR fuel assembly is nominally 1075 g (maximum 1100 g) of uranium enriched to 93% ²³⁵U. Certain plates contain boron carbide (B₄C) mixed with the fuel as a burnable poison to minimize radial power peaking and extend the life cycle of the fuel element. A summary of data about the HEU spent nuclear fuel category is provided in Table 4-2.

Table 4-2. Data Summary for Highly Enriched Uranium Spent Fuel *

Description	Units
Volume (as is)	315 m ³
Mass	63 MT 72 MTHM
Thermal Output (year 2030)**	441 W/m ³
Radionuclide Inventory (year 2030)	4.09 × 10 ⁷ Ci
Uranium Enrichment	80 - 93%

* See also Appendix A. These values are based on information available at the time of analysis and could change in response to new data.
 ** The thermal output values are calculated from the radionuclide inventory.

4. Description of Waste and Waste Parcels

TRI-6342-3752-1

Figure 4-2. Representative highly enriched uranium (HEU) Advanced Test Reactor (ATR) fuel assembly.

4.1.3 Robust, Highly Enriched Uranium Spent Nuclear Fuel (Shippingport)

Shippingport fuel represents the robust, highly enriched uranium spent nuclear fuel category. The Shippingport fuel was a developmental fuel in the DOE Pressurized Water Reactor research program. It was the second of three cores irradiated in the Shippingport Atomic Power Station at Shippingport, Pennsylvania (see Appendix A). The high power density, high total energy core required the development of a fuel element of high loading that would withstand long irradiation exposure at high heat fluxes. The fuel cluster consists of two oxide fuel plate subassemblies welded together to form a square structure and two Zircaloy-4 cluster extensions welded to the ends of the subassemblies (Figure 4-3). A summary of data about the robust, highly enriched spent fuel category is provided in Table 4-3.

Table 4-3. Data Summary for Robust, Highly Enriched Spent Nuclear Fuel *

Description	Units
Volume (as is)	931 m ³
Mass	3780 MT 110 MTHM
Thermal Output (year 2030)**	555 W/m ³
Radionuclide Inventory (year 2030)	1.74×10^8 Ci
Uranium Enrichment	0.3 - 81%

* See also Appendix A. These values are based on information at the time of analysis and could change in response to new data. This category includes fuel stored at INEL from Naval propulsion reactors.
 ** The thermal output values are calculated from the radionuclide inventory.

4.1.4 Low Enriched Uranium (LEU) Spent Nuclear Fuel (PWR Fuel)

The low enriched uranium (LEU) fuel category is represented by a research pressurized water reactor (PWR) fuel. The basic component of a typical PWR fuel assembly is a fuel element (rod), which is a zircaloy sheath containing uranium oxide fuel pellets (Figure 4-4). The diameter of the elements is slightly larger than that of an ordinary pencil. The elements are held in a square array with grid spacers, which are placed at intervals over the length of the elements. The total assembly is 4.0 to 4.5 m. A summary of data about the LEU spent fuel category is provided in Table 4-4.

Table 4-4. Data Summary for Low Enriched Uranium Spent Fuel *

Description	Units
Volume (as is)	167 m ³
Mass	250 MT 162 MTHM
Thermal Output (year 2030)**	470 W/m ³
Radionuclide Inventory (year 2030)	2.07×10^7 Ci
Uranium Enrichment	<10%

* See also Appendix A. These values are based on information at the time of analysis and could change in response to new data.
 ** The thermal output values are calculated from the radionuclide inventory.

4. Description of Waste and Waste Parcels

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Figure 4-3. Representative Shippingport spent nuclear fuel assembly.

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Figure 4-4. Representative low enriched uranium (LEU) Pressurized Water Reactor (PWR) fuel assembly.

4.1.5 Weapons Production Spent Nuclear Fuel (N-Reactor)

The weapons production spent nuclear fuel category is represented by fuel from the N-Reactor fuel, which is currently stored at the Hanford site in Washington state. N-Reactor fuel is metallic uranium (601 alloy) clad with zirconium alloy (Zircaloy-2) (Figure 4-5). Zircaloy-2 is primarily zirconium with about 1% tin and trace quantities of other elements, such as iron, chromium, nickel, and carbon. During fabrication, the uranium core was coextruded with the cladding, which results in an intermetallic layer. Extruded stock was then cut to the fuel element length, and the ends machined, brazed, and welded for final closure. N-Reactor fuel is categorized as either weapon grade or fuel grade, depending on plutonium composition. The ^{240}Pu isotopic content of weapon fuel is less than 6%; the content of fuel grade is equal or greater than 6%. For this performance assessment, however, the inventory is calculated as the total for both weapon and fuel grades; they are not modeled separately. A summary of data about the N-Reactor spent nuclear fuel is provided in Table 4-5.

4.1.6 Calcine High-Level Waste

Two types of calcines are stored at the Chem Plant: aluminum and zirconium calcines.

The aluminum wastes were the first high-level wastes generated (from the dissolution of Materials Test Reactor elements) at the Chem Plant. Use of a fluidized-bed to convert these liquids into a solid form (oxide and fluoride) was first demonstrated in 1963 (Lahey and Bower, 1963). The process used indirect heating to denitrify the acidic, aqueous waste and convert it into a dry, granular solid that was stored in underground bins. In the calcination process, the volume reduction of the wastes was about 8-10:1. The dry solids consist of both a granular material and a powder

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Figure 4-5. Representative N-Reactor spent nuclear fuel assembly.

Table 4-5. Data Summary for Weapons Production Spent Nuclear Fuel *

Description	Units
Volume (as is)	205 m ³
Mass	2300 MT 2100 MTHM
Thermal Output (year 2030)**	470 W/m ³
Radionuclide Inventory (year 2030)	3.03 × 10 ⁷ Ci
Uranium Enrichment	0.9 - 1.25%

* See also Appendix A. These values are based on information available at the time of analysis and could change in response to new data.
 ** The thermal output values are calculated from the radionuclide inventory.

(about 3 to 18 wt%) (Staples et al., 1979); both the granules and powder are pneumatically retrievable and transportable. The granular material ranges in size from 0.2 to 0.5 mm. In terms of short-lived radionuclide concentrates, the aluminum fuels and the resulting wastes provide the highest thermal outputs ("power densities") (W/m³) of any of the wastes processed in the waste calcination facilities at the Chem Plant.

The zirconium waste originated from the processing of U.S. Navy nuclear fuels with their zirconium cladding. The Navy fuel dissolution requires a more complex process, using aqueous hydrofluoric acid to chemically dissolve the fuel assemblies. Aluminum nitrate was blended—first as a cold feed stock and then later as a coprocessing effort—with the zirconium dissolution product to complex the free fluorides. The calcination of zirconium wastes requires the addition of calcium nitrate to form calcium fluoride; all the other components of the waste are converted to their oxide form. Because of the cold chemical addition to the fluoride wastes, liquid to solid volume reduction factors are closer to 6-7:1. The power densities are moderate compared with the aluminum calcines.

Process options for calcine include glass-ceramic, borosilicate, and loose grain solids. A summary of data about the calcine high-level waste is provided in Table 4-6.

Table 4-6. Data Summary for Calcine High-Level Waste*

Description	Units		
	Loose	Glass-Ceramic	Borosilicate
Volume (as is)	4250 m ³	3825 m ³	12750 m ³
Mass	595 MT 320 MTHM*	12240 MT 320 MTHM	33150 MT 320 MTHM
Thermal Output (year 2030)***	9.74 W/m ³	1.28 W/m ³	4.1 W/m ³
Radionuclide Inventory (year 2030)	2.04 × 10 ⁷ Ci	2.04 × 10 ⁷ Ci	2.04 × 10 ⁷ Ci

* See also Appendix A. These values are based on information available at the time of analysis and could change in response to new data.
 ** This value is based on the millions of curies of alpha emitters with half-lives greater than 20 yr, or gamma and beta emitters with half-lives greater than 100 yr in the high-level waste.
 ***The thermal output values are calculated from the radionuclide inventory.

4. Description of Waste and Waste Parcels

4.1.7 Borosilicate Glass High-Level Waste from DOE Sites

Plans call for the borosilicate glass from Savannah River, Hanford, and West Valley to be produced from neutralized high-level waste. The respective containers contain 1682 kg, 1650 kg, and 1900 kg of glass. Because the influence of the mass of glass is minor, 1900 kg was used for all three containers in the performance assessment calculations. The DOE wastes will be accepted as received with one disposal option (i.e., borosilicate glass). A summary of the waste data for the immobilized high-level waste from Savannah River, Hanford, and West Valley is given in Table 4-7.

Table 4-7. Data Summary for Waste from Savannah River, Hanford, and West Valley*

Description	Savannah River	Hanford	West Valley
Volume (as is)	3307 m ³	1227 m ³	193 m ³
Mass	888 MT 8036 MTHM**	3230 MT 1160 MTHM**	523 MT 72 MTHM**
Thermal Output (year 2030)***	375 W/m ³	447 W/m ³	168 W/m ³
Radionuclide Inventory (year 2030)	5.57 × 10 ⁸ Ci	2.63 × 10 ⁸ Ci	1.35 × 10 ⁷ Ci

* See also Appendix A. These values are based on information available at the time of analysis and could change in response to new data.
** This value is based on the millions of curies of alpha emitters with half-lives greater than 20 yr, or gamma and beta emitters with half-lives greater than 100 yr in the high-level waste.
***The thermal output values are calculated from the radionuclide inventory.

4.2 Distribution of Radionuclides in Waste

The inventory of the radionuclides in the waste and the decay chains are presented below.

4.2.1 Radionuclide Inventory

The anticipated radionuclide inventory for the spent fuels and high-level waste under study is provided in Appendix A, Tables A.2.1.2 through A.2.1.10. The anticipated radionuclide inventory is the projected radionuclide inventory of the spent fuel or high-level waste that needs to be disposed of in a repository by the year 2030. Note that for the anticipated high-level waste, all the liquid wastes are assumed to be converted into calcine. Thus, no liquid waste is included in the anticipated inventory.

The fuel radionuclide inventories were derived from ORIGEN (Oakridge Isotope Generation) code runs. Because of the wide variety of fuels considered, some types were grouped together for the purpose of inventory calculations. For example, ORIGEN data were available for highly enriched uranium ATR fuel. Other highly enriched fuels, such as Shippingport fuel, were treated as an equivalent number of ATR elements based on the amount of MTHM. Low-enriched uranium fuels were treated as commercial PWR fuel. ORIGEN runs were available for N-Reactor fuels, which were categorized separately.

The ORIGEN runs available were all performed using high burnup values. These values tended to overstate fission-product inventories because many of the fuels actually had low burnup. The values presented in this report are prorated by burnup (see Appendix A, Section A.2.1).

4.2.2 Radionuclides Considered in 1994 Performance Assessment

All 63 radionuclides shown in Appendix A are considered in the performance assessment (Table 4-8) and were used for the calculations for direct release due to drilling, and the model for heat generation. The initial activities (in curies) of the 63 radionuclides considered for the INEL and DOE wastes are shown in Figure 4-6. Twelve radionuclides were considered in the transport calculations; they include the isotopes of carbon, iodine, neptunium, plutonium, protactinium, radium, selenium, technetium, and uranium. Table 4-9 provides a comparison of the radionuclides selected for transport with the radionuclides whose inventory, normalized to the 40 CFR 191 Table 1 release limit, exceeds values of 0.001, 0.01, 0.1, 1, and 10 during the periods from 100 to 1000 yr and from 1000 to 10,000 yr. The decay of selected radionuclides whose inventory, normalized to the EPA release limits, exceeds values of 0.001, 0.01, 0.1 and 1.0 (see Section 2.3.1) during two periods, 100 to 1000 yr and 1000 to 10,000 yr, is shown in Figure 4-7.

Radionuclide Chains and Half-Lives. A total of 156 radionuclides occur in the decay chains for the spent fuel and high-level waste for the 1994 PA. The decay chains for the 63 radionuclides in the anticipated inventory are shown in Figure 4-8. The half-life for each radionuclide listed in the literature by ICRP Publication 38 (ICRP, 1983) is also shown on Figure 4-8. Daughter radionuclides with extremely short half-lives and which make a small contribution to the curie inventory were omitted in the decay chains.

Waste Unit Factor. For the Containment Requirements of 40 CFR 191, the amount of radionuclides that can be released from the repository is proportional to the amount of radionuclides emplaced. The proportional constant is called a waste unit factor (f_w). The waste unit factor, f_w , that was used in the performance assessment calculations when disposal of waste forms in a group was evaluated (including borosilicate glass from Savannah River, Hanford, and West Valley) is the sum of the following:

1. The amount of the spent fuels (in metric tons of heavy metal [MTHM]), as defined in 40 CFR 191, Appendix A, Note 1(a), divided by 1000
2. The curies of radionuclides of gamma or beta emitters in the high-level waste with half-lives greater than 100 years, or any alpha emitters with half-lives greater than 20 years, as defined by 40 CFR 191, Appendix A, Note 1(d), divided by 1,000,000.

The waste unit factor determined for the 1994 PA is 12.056 (Table 4-10). This waste unit factor was not used in this performance assessment when single waste types were compared (Simple PA).

4.3 Treatment Options for the Waste

Before the waste is placed into a container for disposal, the waste is treated. The purpose of treatment is to make the waste form more resistant to transport in repository groundwater and thus eventual release. The treatments being considered for this performance assessment are minimal treatment for the spent fuel and three treatment options for the calcine high-level waste.

4.3.1 Treatment Options for the Spent Fuel

The 1994 PA selected only one treatment option for spent fuel – minimal treatment – in acknowledgment of time and funding constraints, which prevented an examination of the same five options that had been studied in the 1993 PA. The decision to select minimal treatment was based on a result from the 1993 PA that indicated not only that all five of the treatment options potentially complied with the regulatory criteria under study but also that only the extensive treatment improved performance.

For spent nuclear fuel, the treatment option modeled in the 1994 PA is disposal with either minimal or no treatment, which equates most closely to Option 1 in the 1993 PA. The spent fuel assemblies are packed reasonably tightly into the waste containers, which results in fewer containers than estimated in the draft Environmental Impact

4. Description of Waste and Waste Parcels

Table 4-8. Radionuclides Considered in 1994 Performance Assessment

Element Name	Used In Direct Release and Heat Calculations	Used in Source Term Calculations	Used in Transport Calculations (Simple and Complex PAs)	Allowable Release Rate Based on 10 CFR 60
Americium	²⁴¹ Am ^{242m} Am ²⁴³ Am	²⁴¹ Am ^{242m} Am ²⁴³ Am		5.7516 6.0465×10^{-5} 3.6803×10^{-2}
Barium	^{137m} Ba			3.6823×10^{-7}
Carbon	¹⁴ C	¹⁴ C	¹⁴ C	3.6219×10^{-3}
Cadmium	¹¹³ Cd ^{113m} Cd			2.6673×10^{-15} 2.5687×10^{-23}
Cerium	¹⁴⁴ Ce			0.0
Chlorine	³⁶ Cl			2.6183×10^{-5}
Curium	²⁴³ Cm ²⁴⁴ Cm ²⁴⁵ Cm ²⁴⁶ Cm ²⁴⁷ Cm			4.8446×10^{-14} 1.6803×10^{-16} 1.1226×10^{-5} 1.3413×10^{-6} 1.1448×10^{-12}
Cobalt	⁶⁰ Co			0
Cesium	¹³⁴ Cs ¹³⁵ Cs ¹³⁷ Cs	¹³⁵ Cs ¹³⁷ Cs		0 1.3941×10^{-2} 3.6823×10^{-7}
Europium	¹⁵² Eu ¹⁵⁴ Eu ¹⁵⁵ Eu			6.4658×10^{-24} 2.3696×10^{-33} 0
Iron	⁵⁵ Fe			0
Iodine	¹²⁹ I	¹²⁹ I	¹²⁹ I	2.9888×10^{-4}
Krypton	⁸⁵ Kr			1.5677×10^{-28}
Niobium	^{93m} Nb			1.1782×10^{-1}
Neodymium	¹⁴⁴ Nd			1.0757×10^{-8}
Nickel	⁵⁹ Ni ⁶³ Ni	⁵⁹ Ni ⁶³ Ni		2.3562×10^{-1} 6.4521×10^{-4}
Neptunium	²³⁷ Np	²³⁷ Np	²³⁷ Np	1.9956×10^{-2}
Protactinium	²³¹ Pa	²³¹ Pa	²³¹ Pa	2.2495×10^{-3}
Lead	²¹⁰ Pb			7.3433×10^{-5}
Palladium	¹⁰⁷ Pd			1.9652×10^{-3}
Promethium	¹⁴⁷ Pm			0

Table 4-8. Radionuclides Considered in 1994 Performance Assessment (Continued)

Element Name	Used In Direct Release and Heat Calculations	Used in Source Term Calculations	Used in Transport Calculations (Simple and Complex PAs)	Allowable Release Rate Based on 10 CFR 60
Plutonium	^{238}Pu ^{239}Pu ^{240}Pu ^{241}Pu ^{242}Pu ^{244}Pu	^{238}Pu ^{239}Pu ^{240}Pu ^{241}Pu ^{242}Pu	^{239}Pu	3.2949×10^{-2} 9.2867 1.5135 1.1244×10^{-5} 4.7529×10^{-3} 2.2357×10^{-11}
Radium	^{226}Ra ^{228}Ra	^{226}Ra		7.8156×10^{-5} 4.4942×10^{-5}
Rubidium	^{87}Rb			3.1268×10^{-7}
Ruthenium	^{106}Ru			0
Antimony	^{125}Sb			0
Selenium	^{79}Se	^{79}Se	^{79}Se	1.3963×10^{-2}
Samarium	^{147}Sm ^{151}Sm	^{147}Sm ^{151}Sm		5.0894×10^{-2} 1.6118×10^{-2}
Tin	$^{121\text{m}}\text{Sn}$ ^{126}Sn	^{126}Sn		2.2863×10^{-8} 3.8576×10^{-2}
Strontium	^{90}Sr	^{90}Sr		1.8438×10^{-7}
Technetium	^{99}Tc	^{99}Tc	^{99}Tc	5.1242×10^{-1}
Tellurium	$^{125\text{m}}\text{Te}$			0
Thorium	^{229}Th ^{230}Th ^{232}Th	^{229}Th ^{230}Th		2.2299×10^{-3} 4.2657×10^{-4} 4.4940×10^{-5}
Uranium	^{232}U ^{233}U ^{234}U ^{235}U ^{236}U ^{238}U	^{232}U ^{233}U ^{234}U ^{235}U ^{236}U ^{238}U	^{233}U ^{234}U ^{235}U ^{236}U ^{238}U	8.0519×10^{-7} 2.316×10^{-2} 5.0070×10^{-2} 1.8146×10^{-3} 6.2936×10^{-3} 8.3339×10^{-3}
Yttrium	^{90}Y			1.8443×10^{-7}
Zirconium	^{93}Zr	^{93}Zr		1.1783×10^{-1}
Total Radionuclides	63	32	12	

4. Description of Waste and Waste Parcels

Table 4-9. Comparison of Radionuclides Selected for Transport (for both Simple and Complex PA) with Inventory Exceeding an EPA Normalized Value of 0.1 and 0.01 for 100 to 1000 yr and 1000 to 10,000 yr during 10,000-yr Regulatory Period

Radionuclide with Normalized Inventory								
100 - 1000 yr				1,000 - 10,000 yr				Radionuclides Selected for Transport
>10	>1	>0.1	>0.01	>10	>1	>0.1	>0.01	
			²⁴³ Cm					
	²⁴³ Am	²⁴³ Am	²⁴³ Am		²⁴³ Am	²⁴³ Am	²⁴³ Am	
		^{242m} Am	^{242m} Am					
²⁴¹ Am	²⁴¹ Am	²⁴¹ Am	²⁴¹ Am	²⁴¹ Am	²⁴¹ Am	²⁴¹ Am	²⁴¹ Am	
		²⁴² Pu	²⁴² Pu			²⁴² Pu	²⁴² Pu	
²⁴⁰ Pu	²⁴⁰ Pu	²⁴⁰ Pu	²⁴⁰ Pu	²⁴⁰ Pu	²⁴⁰ Pu	²⁴⁰ Pu	²⁴⁰ Pu	
²³⁹ Pu	²³⁹ Pu	²³⁹ Pu	²³⁹ Pu	²³⁹ Pu	²³⁹ Pu	²³⁹ Pu	²³⁹ Pu	²³⁹ Pu
²³⁸ Pu	²³⁸ Pu	²³⁸ Pu	²³⁸ Pu		²³⁸ Pu	²³⁸ Pu	²³⁸ Pu	
		²³⁸ U	²³⁸ U			²³⁸ U	²³⁸ U	²³⁸ U
		²³⁶ U	²³⁶ U			²³⁶ U	²³⁶ U	²³⁶ U
		²³⁵ U	²³⁵ U			²³⁵ U	²³⁵ U	²³⁵ U
	²³⁴ U	²³⁴ U	²³⁴ U		²³⁴ U	²³⁴ U	²³⁴ U	²³⁴ U
	²³³ U	²³³ U	²³³ U		²³³ U	²³³ U	²³³ U	²³³ U
		²³² U	²³² U					
	²³⁷ Np	²³⁷ Np	²³⁷ Np		²³⁷ Np	²³⁷ Np	²³⁷ Np	²³⁷ Np
			²³² Th				²³² Th	
		²³⁰ Th	²³⁰ Th		²³⁰ Th	²³⁰ Th	²³⁰ Th	
		²²⁹ Th	²²⁹ Th		²²⁹ Th	²²⁹ Th	²²⁹ Th	
		²³¹ Pa	²³¹ Pa			²³¹ Pa	²³¹ Pa	²³¹ Pa
			²²⁷ Ac				²²⁷ Ac	
						²²⁶ Ra	²²⁶ Ra	
							²¹⁰ Pb	
¹⁵¹ Sm	¹⁵¹ Sm	¹⁵¹ Sm	¹⁵¹ Sm			¹⁵¹ Sm	¹⁵¹ Sm	
	¹⁴⁷ Sm	¹⁴⁷ Sm	¹⁴⁷ Sm		¹⁴⁷ Sm	¹⁴⁷ Sm	¹⁴⁷ Sm	
		¹²⁶ Sn	¹²⁶ Sn			¹²⁶ Sn	¹²⁶ Sn	
			^{121m} Sn					
¹³⁷ Cs	¹³⁷ Cs	¹³⁷ Cs	¹³⁷ Cs					
		¹³⁵ Cs	¹³⁵ Cs			¹³⁵ Cs	¹³⁵ Cs	
			¹²⁹ I				¹²⁹ I	¹²⁹ I
			¹⁰⁷ Pd				¹⁰⁷ Pd	
		⁹⁹ Tc	⁹⁹ Tc			⁹⁹ Tc	⁹⁹ Tc	⁹⁹ Tc
		⁹³ Zr	⁹³ Zr			⁹³ Zr	⁹³ Zr	
⁹⁰ Sr	⁹⁰ Sr	⁹⁰ Sr	⁹⁰ Sr					
		⁷⁹ Se	⁷⁹ Se			⁷⁹ Se	⁷⁹ Se	⁷⁹ Se
	⁶³ Ni	⁶³ Ni	⁶³ Ni					
	⁵⁹ Ni	⁵⁹ Ni	⁵⁹ Ni		⁵⁹ Ni	⁵⁹ Ni	⁵⁹ Ni	
		¹⁴ C	¹⁴ C			¹⁴ C	¹⁴ C	¹⁴ C
7	14	30	35	3	12	25	30	12

TRI-6342-4460-0

(a)

Figure 4-6. Initial (year 2030) activity of 63 radionuclides considered in the performance assessment for (a) graphite spent nuclear fuel, (b) highly enriched uranium spent nuclear fuel, (c) Shippingport spent nuclear fuel, (d) low-enriched uranium spent nuclear fuel, (e) N-Reactor spent fuel, (f) calcine high-level waste, (g) high-level waste from Savannah River, (h) high-level waste from Hanford, (i) high-level waste from West Valley, and (j) total for all nine waste types.

4. Description of Waste and Waste Parcels

(b)

Radionuclides

TRI-6342-4461-0

Figure 4-6.

Initial (year 2030) activity of 63 radionuclides considered in the performance assessment for (a) graphite spent nuclear fuel, (b) highly enriched uranium spent nuclear fuel, (c) Shippingport spent fuel, (d) low-enriched uranium spent nuclear fuel, (e) N-Reactor spent fuel, (f) calcine high-level waste, (g) high-level waste from Savannah River, (h) high-level waste from Hanford, (i) high-level waste from West Valley, and (j) total for all nine waste types (continued).

Figure 4-6. Initial (year 2030) activity of 63 radionuclides considered in the performance assessment for (a) graphite spent nuclear fuel, (b) highly enriched uranium spent nuclear fuel, (c) Shippingport spent fuel, (d) low-enriched uranium spent nuclear fuel, (e) N-Reactor spent fuel, (f) calcine high-level waste, (g) high-level waste from Savannah River, (h) high-level waste from Hanford, (i) high-level waste from West Valley, and (j) total for all nine waste types (continued).

4. Description of Waste and Waste Parcels

TRI-6342-4463-0

(d)

Figure 4-6. Initial (year 2030) activity of 63 radionuclides considered in the performance assessment for (a) graphite spent nuclear fuel, (b) highly enriched uranium spent nuclear fuel, (c) Shippingport spent nuclear fuel, (d) low-enriched uranium spent nuclear fuel, (e) N-Reactor spent fuel, (f) calcine high-level waste, (g) high-level waste from Savannah River, (h) high-level waste from Hanford, (i) high-level waste from West Valley, and (j) total for all nine waste types (continued).

(e)

Radionuclides

TRI-6342-4464-0

Figure 4-6.

Initial (year 2030) activity of 63 radionuclides considered in the performance assessment for (a) graphite spent nuclear fuel, (b) highly enriched uranium spent nuclear fuel, (c) Shippingport spent fuel, (d) low-enriched uranium spent nuclear fuel, (e) N-Reactor spent fuel, (f) calcine high-level waste, (g) high-level waste from Savannah River, (h) high-level waste from Hanford, (i) high-level waste from West Valley, and (j) total for all nine waste types (continued).

4. Description of Waste and Waste Parcels

TRI-6342-4465-0

(f)

Figure 4-6. Initial (year 2030) activity of 63 radionuclides considered in the performance assessment for (a) graphite spent nuclear fuel, (b) highly enriched uranium spent nuclear fuel, (c) Shippingport spent fuel, (d) low-enriched uranium spent nuclear fuel, (e) N-Reactor spent fuel, (f) calcine high-level waste, (g) high-level waste from Savannah River, (h) high-level waste from Hanford, (i) high-level waste from West Valley, and (j) total for all nine waste types (continued).

TRI-6342-4466-0

(g)

Figure 4-6. Initial (year 2030) activity of 63 radionuclides considered in the performance assessment for (a) graphite spent nuclear fuel, (b) highly enriched uranium spent nuclear fuel, (c) Shippingport spent fuel, (d) low-enriched uranium spent nuclear fuel, (e) N-Reactor spent fuel, (f) calcine high-level waste, (g) high-level waste from Savannah River, (h) high-level waste from Hanford, (i) high-level waste from West Valley, and (j) total for all nine waste types (continued).

4. Description of Waste and Waste Parcels

(h)

Figure 4-6.

Initial (year 2030) activity of 63 radionuclides considered in the performance assessment for (a) graphite spent nuclear fuel, (b) highly enriched uranium spent nuclear fuel, (c) Shippingport spent fuel, (d) low-enriched uranium spent nuclear fuel, (e) N-Reactor spent fuel, (f) calcine high-level waste, (g) high-level waste from Savannah River, (h) high-level waste from Hanford, (i) high-level waste from West Valley, and (j) total for all nine waste types (continued).

TRI-6342-4468-0

(i)

Figure 4-6. Initial (year 2030) activity of 63 radionuclides considered in the performance assessment for (a) graphite spent nuclear fuel, (b) highly enriched uranium spent nuclear fuel, (c) Shippingport spent nuclear fuel, (d) low-enriched uranium spent nuclear fuel, (e) N-Reactor spent fuel, (f) calcine high-level waste, (g) high-level waste from Savannah River, (h) high-level waste from Hanford, (i) high-level waste from West Valley, and (j) total for all nine waste types (continued).

4. Description of Waste and Waste Parcels

TRI-6342-4469-0

(j)

Figure 4-6. Initial (year 2030) activity of 63 radionuclides considered in the performance assessment for (a) graphite spent nuclear fuel, (b) highly enriched uranium spent nuclear fuel, (c) Shippingport spent fuel, (d) low-enriched uranium spent nuclear fuel, (e) N-Reactor spent fuel, (f) calcine high-level waste, (g) high-level waste from Savannah River, (h) high-level waste from Hanford, (i) high-level waste from West Valley, and (j) total for all nine waste types (continued).

TRI-6342-4412-0

(a)

Figure 4-7. Normalized activity decay history of individual radionuclides that exceed a normalized release of (a) 0.001 during 100 to 1000 yr, (b) 0.001 during 1000 to 10,000 yr, (c) 0.01 during 100 to 1000 yr, (d) 0.01 during 1000 to 10,000 yr, (e) 0.1 during 100 to 1000 yr, (f) 0.1 during 1000 to 10,000 yr, (g) 1.0 during 100 to 1000 yr, and (h) 1.0 during 1000 to 10,000 yr, based on 40 CFR 191 criterion.

4. Description of Waste and Waste Parcels

TRI-6342-4413-0

(b)

Figure 4-7. Normalized activity decay history of individual radionuclides that exceed a normalized release of (a) 0.001 during 100 to 1000 yr, (b) 0.001 during 1000 to 10,000 yr, (c) 0.01 during 100 to 1000 yr, (d) 0.01 during 1000 to 10,000 yr, (e) 0.1 during 100 to 1000 yr, (f) 0.1 during 1000 to 10,000 yr, (g) 1.0 during 100 to 1000 yr, and (h) 1.0 during 1000 to 10,000 yr, based on 40 CFR 191 criterion (continued).

TRI-6342-4414-0

(c)

Figure 4-7. Normalized activity decay history of individual radionuclides that exceeded a normalized release of (a) 0.001 during 100 to 1000 yr, (b) 0.001 during 1000 to 10,000 yr, (c) 0.01 during 100 to 1000 yr, (d) 0.01 during 1000 to 10,000 yr, (e) 0.1 during 100 to 1000 yr, (f) 0.1 during 1000 to 10,000 yr, (g) 1.0 during 100 to 1000 yr, and (h) 1.0 during 1000 to 10,000 yr, based on 40 CFR 191 criterion (continued).

4. Description of Waste and Waste Parcels

TRI-6342-4415-0

(d)

Figure 4-7. Normalized activity decay history of individual radionuclides that exceed a normalized release of (a) 0.001 during 100 to 1000 yr; (b) 0.001 during 1000 to 10,000 yr; (c) 0.01 during 100 to 1000 yr; (d) 0.01 during 1000 to 10,000 yr; (e) 0.1 during 100 to 1000 yr; (f) 0.1 during 1000 to 10,000 yr; (g) 1.0 during 100 to 1000 yr; and (h) 1.0 during 1000 to 10,000 yr, based on 40 CFR 191 criterion (continued).

TRI-6342-4416-0

(e)

Figure 4-7. Normalized activity decay history of individual radionuclides that exceed a normalized release of (a) 0.001 during 100 to 1000 yr, (b) 0.001 during 1000 to 10,000 yr, (c) 0.01 during 100 to 1000 yr, (d) 0.01 during 1000 to 10,000 yr, (e) 0.1 during 100 to 1000 yr, (f) 0.1 during 1000 to 10,000 yr, (g) 1.0 during 100 to 1000 yr, and (h) 1.0 during 1000 to 10,000 yr, based on 40 CFR 191 criterion (continued).

4. Description of Waste and Waste Parcels

TRI-6342-4417-0

(f)

Figure 4-7. Normalized activity decay history of individual radionuclides that exceed a normalized release of (a) 0.001 during 100 to 1000 yr, (b) 0.001 during 1000 to 10,000 yr, (c) 0.01 during 100 to 1000 yr, (d) 0.01 during 1000 to 10,000 yr, (e) 0.1 during 100 to 1000 yr, (f) 0.1 during 1000 to 10,000 yr, (g) 1.0 during 100 to 1000 yr, and (h) 1.0 during 1000 to 10,000 yr, based on 40 CFR 191 criterion (continued).

(g)

(h)

Figure 4-7. Normalized activity decay history of individual radionuclides that exceed a normalized release of (a) 0.001 during 100 to 1000 yr, (b) 0.001 during 1000 to 10,000 yr, (c) 0.01 during 100 to 1000 yr, (d) 0.01 during 1000 to 10,000 yr, (e) 0.1 during 100 to 1000 yr, (f) 0.1 during 1000 to 10,000 yr, (g) 1.0 during 100 to 1000 yr, and (h) 1.0 during 1000 to 10,000 yr, based on 40 CFR 191 criterion (continued).

4. Description of Waste and Waste Parcels

Figure 4-8. Radionuclide decay chains considered for spent fuel and high-level waste for complementary cumulative distribution function (CCDF) development (63 of the possible 156 radionuclides).

TRI-6342-5007-0

Figure 4-8. Radionuclide decay chains considered for spent fuel and high-level waste for complementary cumulative distribution function (CCDF) development (63 of the possible 156 radionuclides) (continued).

4. Description of Waste and Waste Parcels

TRI-6342-5008-0

Figure 4-8. Radionuclide decay chains considered for spent fuel and high-level waste for complementary cumulative distribution function (CCDF) development (63 of the possible 156 radionuclides) (continued).

Note: All Half-Lives Shown in Years

TRI-6342-5009-0

Figure 4-8. Radionuclide decay chains considered for spent fuel and high-level waste for complementary cumulative distribution function (CCDF) development (63 of the possible 156 radionuclides) (continued).

4. Description of Waste and Waste Parcels

Table 4-10. Units of Waste for the INEL PA, Based on 40 CFR 191, Appendix A

Contributing DOE Complexes	Alpha Nuclides >20 yr; Beta and Gamma Nuclides >100 yr (curies)	Units of Waste Based on Note 1(a)*,**	Units of Waste Based on Note 1(d)*,***
<hr/>			
INEL			
Graphite fuel	N/A	0.028	N/A
HEU	N/A	0.072	N/A
Shippingport	N/A	0.110	N/A
LEU		0.1620	N/A
N-Reactor	N/A	2.100	N/A
Calcine	3.20×10^5	N/A	0.320
Savannah River	8.04×10^6	N/A	8.036
Hanford	1.16×10^6	N/A	1.160
West Valley	7.15×10^4	N/A	0.072
		<hr/>	
TOTAL		2.472	9.588
Waste Unit Factor =		12.060	
<hr/>			

* No correction was made for low burnup of some of the highly enriched fuels.

** From 40 CFR 191, Appendix A; the amount of spent fuel, divided by 1000 metric tons of heavy metal.

***From 40 CFR 191, Appendix A; the curies of gamma or beta emitters with a half-life greater than 100 yr, or alpha emitters with a half-life greater than 20 yr, divided by 10^6 .

Statement for spent nuclear fuel management at INEL (U.S. DOE, 1994).^{*} The condition of the graphite spent fuel (Fort St. Vrain), robust, highly enriched, zircaloy-clad spent fuel (Shippingport), and low-enriched spent fuel (PWR fuel) is good enough that these wastes can be placed directly into handling containers for storage and eventual disposal. Some of the highly enriched spent fuel (aluminum-clad ATR fuel) was damaged from corrosion during storage in water basins. The current plan for the ATR fuel is to dry the assemblies, arrest corrosion, and then place the assemblies into stainless steel capsules. The capsules could then be placed in handling containers and into dry storage awaiting transport to a disposal system. Because the weapons production fuel (zircaloy-clad N-Reactor fuel) was often damaged when forcibly ejected from the reactor core, some type of drying and stabilization may be required for the N-Reactor fuel; however, no final plans are available at this time. Hence, the assumption was made that only drying and stabilization were necessary before the fuel was placed in the handling container for storage and eventual disposal. The heat from oxidizing all the uranium metal in the N-Reactor is about 1.34×10^{10} kJ or only one-tenth the heat energy produced in one year by all the waste in the 12,060 MTHM repository. Future studies can assess the improvement in performance of any treatment for all fuel or only damaged fuel.

4.3.2 Treatment Options for Calcine High-Level Waste

Three treatment options are modeled for the calcined high-level waste from INEL: (1) glass-ceramic, (2) borosilicate glass, and (3) loose, granular solid. Glass-ceramic waste forms use various glass-forming additives and reactants to form the final product. The final treatment process employs temperatures up to 1325 K (1050°C) and pressures ranging from 6.9×10^7 to 1.4×10^8 Pa in the HIP process. The advantage of the HIP process over borosilicate glass is improved volume reduction (higher waste loading), because fewer minerals without entrained radionuclides ("inerts") such as silica are formed. For borosilicate glass, the low calcine loading relative to the quantity of additives needed to make the borosilicate glass results in a significant volume increase. Furthermore, laboratory

* The container for the highly enriched uranium fuel is assumed to have neutron absorbers in the fuel support structure, as explained in Section 4.4.

leach rate testing has demonstrated slightly better results for the glass-ceramic; while leaching of radionuclides from the glass is similar to borosilicate glass, leaching from the crystalline ceramic is better. The different alteration rates for the two encapsulating matrices in the glass-ceramic are included in the source term submodel (see Chapter 11).

The high-level waste from the three DOE sites is always modeled as a borosilicate glass waste form.

4.4 Waste Containers

Three waste handling containers are modeled in the 1994 PA: 125-ton multi-purpose canisters (MPCs), 25-ton legal weight truck (LWT) canisters, and standard canisters for DOE high-level waste (Figure 4-9). The MPCs are used for horizontal emplacement of the waste; LWT containers are used for vertical emplacement of the waste in this performance assessment; DOE standard containers are used in both horizontal and vertical emplacement. (See Chapter 6 for a discussion of horizontal and vertical emplacement.) The MPC is intended to be a handling container that can be used for storage, transportation and disposal. It is currently being considered by the Yucca Mountain Project (see Appendix F).

Up to two disposal containers are modeled: a 100-mm carbon steel outer barrier and a 20-mm Incoloy Alloy 825 inner barrier. One set of calculations did not use the Incoloy Alloy 825 layer.

4.4.1 Multi-Purpose Canisters (MPCs) for Horizontal Emplacement

In the 1994 PA, two sizes of MPCs are used for horizontal emplacement: one for spent fuel and the other for defense high-level waste. The first, SF-MPC (spent fuel MPC) has an outside diameter of 1.77 m and a length of 5.14 m (measurements include disposal containers). The second, DHLW-MPC (defense high-level waste MPC), contains four DHLW canisters and has an outside diameter of 1.84 m and a length of 3.7 m. The MPC is made of 2.54-mm 304L stainless steel. The MPC is overpacked with an inner barrier disposal container of 20-mm corrosion-resistant material (Incoloy Alloy 825), and an outer disposal container of 100-mm carbon steel. The atmosphere inside the container is assumed to be helium.

The MPC is expected to be transported on a rail system; each MPC is placed on an emplacement cart and then "parked" in a disposal room. (See Chapter 6 for a discussion of the waste emplacement orientations.)

Figure 4-10 is an example of the disposal configurations for the graphite fuel in the MPC, including fuel support structures, configuration, number of elements, number of layers, and total numbers of elements for each fuel type.

4.4.2 Legal Weight Truck (LWT) Containers for Vertical Emplacement

The 25-ton LWT is a rectangular container with a length of approximately 457 cm and a 47-cm square top. Figure 4-9 shows the conceptual design for the LWT. The LWT contains a 9.5-mm-thick stainless steel handling container. The atmosphere inside the container is assumed to be helium. Like the MPC, the LWT is overpacked with a 20-mm Incoloy Alloy 825 inner disposal container and an outer disposal container of 100-mm carbon steel.

The LWTs will be transported to the repository and then emplaced in vertical boreholes in the waste disposal room floor. (See Chapter 6 for a discussion of the waste emplacement orientations.)

Figure 4-10 is an example of the disposal configurations for the graphite fuel in the LWT, including fuel support structures, configuration, number of elements, number of layers, and total numbers of elements for each fuel type.

4. Description of Waste and Waste Parcels

25-Ton Legal Weight Truck (LWT) Canister
with Disposal Overpack Containers

"Standard" Canister for DOE
HLW (Container Placed in Disposal
Overpack Composed of Same
Layers as LWT)

(a) Vertical Emplacement

125-Ton Multi-Purpose Canister (MPC) with Disposal Overpack Containers

(b) Horizontal Emplacement

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Figure 4-9. Legal Weight Truck (LWT) canister, Standard Canister for DOE, and Multi-Purpose Canister (MPC) with disposal overpack containers used in 1994 PA.

5 Fort St. Vrain
Fuel Elements
Contained in
0.635 cm
(0.25 in) Thick
Stainless Steel
Basket with
0.635 cm
(0.25 in)
Clearance
in between
Basket and Fuel

Stainless Steel
Basket used
in Both MPC
and LWT

Scale
0 20 40 cm
0 8 16 in

WP 201 - LWT Vertical Emplacement
(5 Layers)

WP 101 - MPC Horizontal Emplacement
(5 Layers)

TRI-6342-4297-0

Figure 4-10. Container loading configurations for graphite fuel.

4.4.3 DOE Standard Container for Horizontal/Vertical Emplacement

The standard container for the high-level waste is 3.0 m long, with a 0.61 m outside diameter (Figure 4-9). The container is made of 9.5-mm 304L stainless steel. For horizontal emplacement, four standard DOE containers are placed in the DHLW-MPC. For vertical emplacement, handling containers of calcine high-level waste from INEL are placed in DOE standard containers, overpacked with the Incoloy Alloy 825 and carbon steel disposal containers, and then into boreholes. Containers of DOE borosilicate glass waste, however, which serve as a reference case, are placed directly into the borehole so that their performance can be compared to results from the 1993 PA.

It should be noted that the conceptual design for the Yucca Mountain Project includes a 100-mm corrosion-resistant layer of 70-30 Cupronickel alloy in place of the carbon steel for the borosilicate glass waste form. This layer was proposed because preliminary experiments indicated that silica glass showed higher alteration rates in the presence of iron. However, the Cupronickel layer is replaced with the standard carbon steel layer in the 1994 PA, in large part so that a common basis of comparison can be maintained among the containers. Other factors that contributed to the decision were that the distribution range for the silica glass dissolution is already four orders of magnitude; the increase in solubility of the glass could not be determined without further evaluation of data; and, finally, the understanding that iron has a potentially beneficial effect in that it can make the chemical environment inside the container reducing for a very long time, thus lowering the solubility of Np and some other actinides. It was beyond the scope of the 1994 PA to examine these competing effects.

4.5 Description of Waste Parcels

The waste parcel is defined as the waste form (i.e., treated waste type), handling container, and disposal container(s) (overpack). The handling container encloses the waste form, and the disposal containers provide structural reinforcement and corrosion resistance. Container materials are described in Section 4.5 above.

4.5.1 Waste Types in Parcels

Twenty-two waste parcels were modeled in the 1994 PA: 11 for horizontal emplacement and 11 for vertical emplacement (Table 4-11). The 11 waste parcels include the five spent fuels, three treatments for INEL calcine waste, and three DOE high-level waste parcels. The difference between the waste parcels for the horizontal and vertical emplacements are the type of container used and, therefore, the amount of waste per waste parcel.

4.5.2 Waste Parcels for Simple and Complex PAs

All 11 parcels per emplacement scheme are modeled in the Simple PA, where each waste type is placed individually into the repository. The waste disposal group for the Complex PA includes nine waste parcels: five spent fuel parcels, one INEL calcine parcel as a glass-ceramic waste form, and three DOE high-level waste parcels. The wastes are assumed to be equally distributed among the waste disposal rooms.

4.5.3 Thermal Power by Waste Parcels

Thermal power is shown in Figure 4-11 for all 22 waste parcels, based on a total of 63 selected radionuclides. The 63 radionuclides were selected based on the half-life or significant contribution to waste parcel activity (see Section 4.2).

Table 4-11. Waste Parcels Modeled in the 1994 Complex and Simple PAs

Waste Parcel ID	Waste Type	Treatment Option	Container	Modeled In	
				Complex PA	Simple PA
Horizontal					
101	Graphite	Whole block	USF-MPC ^a	•	•
102	N-Reactor	Whole block	USF-MPC	•	•
103	Shippingport	Whole block	USF-MPC	•	•
104	ATR (HEU)	Stainless steel capsules	USF-MPC	•	•
105	PWR (LEU)	Whole block	PWR-MPC ^b	•	•
106	INEL calcine	Glass ceramic	DHLW-MPC ^c	•	•
107	Savannah River	Borosilicate glass	DHLW-MPC	•	•
108	Hanford	Borosilicate glass	DHLW-MPC	•	•
109	West Valley	Borosilicate glass	DHLW-MPC	•	•
110	INEL calcine	Borosilicate glass	DHLW-MPC		•
111	INEL calcine	Loose, granular	DHLW-MPC		•
Vertical					
201	Graphite	Whole block	LWT ^d	•	•
202	N-Reactor	Whole block	LWT	•	•
203	Shippingport	Whole block	LWT	•	•
204	ATR (HEU)	Stainless steel capsules	LWT	•	•
205	PWR (LEU)	Whole block	LWT	•	•
206	INEL calcine	Glass ceramic	DOE standard canister	•	•
207	Savannah River	Borosilicate glass	DOE standard canister	•	•
208	Hanford	Borosilicate glass	DOE standard canister	•	•
209	West Valley	Borosilicate glass	DOE standard canister	•	•
210	INEL calcine	Borosilicate glass	DOE standard canister		•
211	INEL calcine	Loose, granular	DOE standard canister		•

^a USF-MPC – 125-ton multi-purpose canister for uncanistered spent fuel^b PWR-MPC – 125-ton multi-purpose canister for commercial fuel^c DHLW-MPC – 125-ton multi-purpose canister for defense high-level waste^d LWT – 25-ton legal weight truck container

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(a)

TRI-6342-4407-0

(b)

Figure 4-11. Thermal power of waste parcels at time of emplacement (year 2030) accounting for 63 radionuclides for (a) waste parcels for horizontal emplacement and (b) waste parcels for vertical emplacement.

4.5.4 Curie Content by Waste Parcel

The curie content of individual waste parcels for the 63 radionuclides is shown in Figure 4-12.

4.5.5 Fissile Mass Contents per Waste Parcel

The fissile mass per waste parcel for the waste group modeled in the Complex PA is shown in Table 4-12 for both the vertical and horizontal emplacements. From the data in Table 4-12, the equivalent MTHM (total fissile mass of ^{233}U , ^{235}U , ^{239}Pu and ^{241}Pu) can be computed for the spent fuel waste parcels. The equivalent MTHM (1 MTHM = 1 kg) is 0.874 for graphite spent fuel, 40.12 for highly enriched uranium spent fuel (ATR), 35.39 for robust highly enriched uranium spent fuel (Shippingport), 2.752 for low-enriched uranium spent fuel (PWR), and 18.63 for weapons production fuel (N-Reactor). The fissile mass contents for all waste parcels (101 to 111; 201 to 211) are provided in Appendix F, Tables F-24 and F-25.

4.6 Summary of Modeling Assumptions for Waste Forms and Waste Parcels

- Disposal of the waste inventory into an unsaturated tuff geologic repository is assumed to occur in the year 2030.
- The initial inventory of 63 radionuclides is considered for the direct release from drilling model, and the heat generation model. Thirty-two radionuclides are considered for the source term submodel for groundwater release. Twelve radionuclides are considered for transport in the groundwater.
- Minimal treatment options are considered for the spent fuel types.
- Calcine high-level waste from INEL is assumed to be a glass-ceramic waste form in the Complex PA; calcine is modeled as glass-ceramic, borosilicate glass, and a loose grain solid for the Simple PA.
- The high-level waste from the three DOE sites is borosilicate glass.
- The 125-ton MPC, overpacked with two disposal containers, is used for horizontal, indrift emplacement.
- The 25-ton LWT canister, overpacked with two disposal containers, is used for vertical, borehole emplacement for the spent fuel assemblies.
- For vertical emplacement of INEL high-level waste, the DOE standard canisters are placed in an LWT and then emplaced in the vertical borehole. For DOE high-level waste, the DOE standard canister is directly emplaced in the vertical borehole.
- Four standard canisters of INEL and DOE high-level waste are placed in a DHLW-MPC for horizontal emplacement.
- The handling container for the LWT and DOE standard container is 9.5-mm stainless steel; for the MPC, it is 25.4-mm stainless steel.
- The inner disposal container is 20-mm Incoloy Alloy for the MPC, LWT, and DOE standard canister.
- The outer disposal container is 100-mm carbon steel for the MPC, LWT, and DOE standard canister.

4. Description of Waste and Waste Parcels

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(a)

TRI-6342-4409-0

(b)

Figure 4-12. Curie content of waste parcels based on initial inventory of 63 radionuclides at time of emplacement (year 2030) for (a) waste parcels for horizontal emplacement and (b) waste parcels for vertical emplacement.

Table 4-12. Fissile Mass per Waste Parcel for Vertical and Horizontal Emplacement

Waste Parcel ID	Description	Number of Waste Parcels Required in Complex PA*	Fissile Mass (kg)				
			²³³ U	²³⁵ U	²³⁹ Pu	²⁴¹ Pu	Total
Horizontal Emplacement							
101	USF-MPC: Graphite SNF	83	2.869e+00	7.643e+00	2.218e-02	0.000e+00	1.053e+01
102	USF-MPC: N-Reactor (Hanford) SNF	59	3.226e-07	2.575e+02	5.792e+01	3.605e-01	3.158e+02
103	USF-MPC: Shippingport SNF	256	1.067e-05	1.367e+02	1.464e+00	7.778e-02	1.382e+02
104	USF-MPC: ATR (HEU) SNF	33	4.928e-05	9.267e+02	2.891e+02	3.401e-02	1.216e+03
105	PWR-MPC: Commercial PWR (LEU) SNF	36	3.329e-05	4.582e+01	2.895e+01	1.660e+00	7.643e+01
106	HLWG-MPC: INEL Calcine Glass-Ceramic HLW	2037	1.689e-04	1.138e-01	2.820e-02	0.000e+00	1.422e-01
107	HLWG-MPC: DOE Savannah River HLW	1321	6.544e-07	2.910e-01	8.306e-01	6.483e-02	1.186e+00
108	HLWG-MPC: DOE Hanford Reservation HLW	490	0.000e+00	3.646e-01	9.076e-02	1.002e-03	4.654e-01
109	HLWG-MPC: DOE West Valley HLW	69	1.462e-02	6.528e-01	4.097e-01	1.227e-02	1.089e+00
Vertical Emplacement							
201	LWT: Graphite SNF	560	4.253e-01	1.133e+00	3.287e-03	0.000e+00	1.561+00
202	LWT: N-Reactor (Hanford) SNF	394	4.830e-08	3.857e+01	8.674e+00	5.399e-02	4.729e+01
203	LWT: Shippingport SNF	1540	1.773e-06	2.272e+01	2.434e-01	1.293e-02	2.298e+01
204	LWT: ATR (HEU) SNF	233	6.980e-06	1.312e+02	4.094e+01	4.817e-03	1.722e+02
205	LWT: Commercial PWR (LEU) SNF	252	4.756e-06	6.456e+00	4.136e+00	2.372e-01	1.092e+01
206	DOESC: INEL Calcine Glass-Ceramic HLW	8147	4.223e-05	2.845e-02	7.051e-03	0.000e+00	3.555e-02
207	DOESC: DOE Savannah River HLW	5283	1.636e-07	7.277e-02	2.077e-01	1.621e-02	2.967e-01
208	DOESC: DOE Hanford Reservation HLW	1960	0.000e+00	9.115e-02	2.269e-02	2.505e-04	1.141e-01
209	DOESC: DOE West Valley HLW	276	3.655e-03	1.632e-01	1.024e-01	3.067e-03	2.724e-01
* See Chapter 7 for description of Complex PA.							

5. Hypothetical Geologic Barrier

K. F. Brinster, M. L. Wilson, and R. P. Rechard

Characteristics of the hypothetical geologic barrier – volcanic tuff – are summarized in this chapter. The description focuses on the major concepts and features of the barrier as they relate to the conceptual model for the performance assessment. Presented in this chapter are general criteria for site selection, specific characteristics of tuffs, a stratigraphic description of the site, a discussion of climatic changes and how these changes affect the hydrology, and a description of flow modeling parameters and assumptions.

5.1 Volcanic Tuff as Geologic Barrier (K. F. Brinster)

Geologic media of several different origins have been considered as regional barriers for the disposal of spent nuclear fuel and high-level radioactive waste. These rocks—granite, salt, basalt, and tuff—all have different geologic, geomechanical, and geochemical characteristics that can influence the overall design of a repository system. Some of the most important geologic variables to be considered in locating a waste disposal facility within any deep geologic medium are hydrologic properties such as permeability, porosity, and storativity; the local and regional groundwater flow field for assessing the long-term flow and transport of waste from a breached repository; and thermal, transport, and mechanical properties since, for decades after emplacement, the decay of radionuclides generates heat that can drive fluid flow and create thermal and geomechanical stresses.

Three main criteria are considered during selection of a site for radioactive waste disposal. The first criterion evaluates land-use conflicts (both human and natural), the second studies the technical suitability of the site, and third examines how well the waste can be isolated from the human population (Carter, 1987). In this performance assessment only the latter two were considered because the site is hypothetical and assumed to have met the first criterion.

5.1.1 Technical Suitability

The technical suitability of a site is determined by how easily the rock can be mined, how impervious the rocks are to water, present and future mechanical and chemical conditions of the rock, and the ability of the site to provide reasonable isolation of the waste from the biosphere. The geologic media of a candidate repository site should possess simple hydrological and geologic elements. Thus, the site should be

1. Massive, competent, uniform, and largely unfractured.
2. Tectonically stable and relatively unfaulted.
3. Geomorphically consistent and predictable.
4. Hydrologically separated from the waste to keep dissolution and transport at a minimum.
5. Non-reactive with the waste so as not to pose a threat to humans.

The ability to retrieve waste may also be a criterion; retrievability would require underground openings that are stable enough to make backfilling with crushed rock unnecessary.

5.1.2 Reasonable Isolation

The site must also meet the criterion of providing reasonable isolation of the waste from the biosphere, especially the human population. To satisfy this criterion, site characteristics in terms of hydrology, tectonics, chemistry, and geology must be considered with regard to whether they are conducive to isolation. Reasonable isolation could also be accomplished by ensuring that the waste containers are long-lived, thus making siting possible in a variety of geologic and geographic environments (Carter, 1987). The primary consideration of this criterion in the current performance assessment was to specify burial at sufficient thickness and depth in the geologic media.

5.1.3 Advantages and Disadvantages of Tuff Deposits

Certain characteristics of tuff provide particular advantages and disadvantages for a disposal system for radioactive waste. The advantages are

- Some altered tuffs provide a high sorptive barrier to radionuclide migration.
- Many tuff sites are geographically isolated from population centers.
- Many sites have little land use competition.
- Groundwater is likely to be saturated with respect to silica, which readily combines with uranium to form uranosilicates.
- Waste can be easily retrieved.
- Site is easily mined.

In addition, the site at Yucca Mountain offers two advantages in particular:

- Proximity to the Nevada Test Site, which is already federally regulated land (U.S. DOE, 1988a).
- Aridity of the region coupled with a thick unsaturated layer to ensure that minimal moisture will come in contact with the waste.

The disadvantages are as follows:

- The highly fractured nature of tuff increases the potential for short groundwater travel times.
- Excavation activities may increase permeability of the tuff around the repository.
- The normal chemical environment is potentially oxidizing if flow through the mountain is high.
- Releases of radioactive gases, such as "CO₂," can move rapidly to the environment because upward air flow is promoted by the high porosity of tuff and thermal buoyancy. (This characteristic is recognized as a disadvantage only when results are compared to criteria from 40 CFR 191.)

5.1.4 Origin and Occurrence of Tuff Deposits

Tuff is an extrusive igneous rock. It is formed by the eruption or extrusion of magma (commonly molten rock with some entrained, early formed crystals and fragments of partially dissolved to intact rock from the wall of the eruptive conduit). At the surface, the extruded magma is called lava. The resulting rock is called tuffaceous, if it is erupted as variously sized particles from large, often explosive vents, forming pyroclastic (literally "fire fragment") ash falls or ash flows.

Because igneous rocks are comprised of a wide range of minerals as well as noncrystalline glass in some cases, the composition of most igneous rocks is most easily presented as percentages of metal oxides, with silica (silicon dioxide, SiO₂) predominant in most rocks. Silica content ranges from about 35 to 80 weight percent silica. Most extensive deposits of tuff are high in silica (rhyolitic) and formed from very viscous magmas. This high viscosity tends to retain volatile compounds that separate from the magma as it rises in the earth's crust. When the pressure in the gas-charged magma reaches lithostatic pressure, the magma is disrupted, producing the explosive volcanic eruptions characteristic of these magmas. The deposition of these pyroclastic fragments produces deposits consisting of tuff, ash, cinders, and blocks or bombs, in order of increasing size of the fragments. Finer-grained tuffs may be classified according to the proportions of glass, crystals, and entrained rock fragments (Figure 5-2). They may also be classified according to the proportions of vitric (glassy) tuff and crystalline tuff fragments (Figure 5-3).

Ejecta from a volcano may consist of old material from the throat and walls of the vent, new magma, or deep-seated country rock. Tuff deposits such as the ones at Yucca Mountain are composites that consist of ash-fall tuffs, ash-flow tuffs, and reworked tuffs. Ash-fall tuffs form from airborne ejecta of volcanos, which form relatively unconsolidated, generally thin deposits whose grain size decreases away from the vent. Waterborne deposits of reworked tuff are commonly bedded, and better sorted than air-fall deposits, and may have been commingled with other sedimentary material. Ash-flow deposits result from the collapse of an eruptive pyroclastic cloud. As the cloud collapses,

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Figure 5-1. Location of tuff deposits in the Basin and Range Province.

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Figure 5-2. Subdivisions of tuff, according to composition of fragments (after Pettijohn, 1975).

5. Hypothetical Geologic Barrier

Figure 5-3. Nomenclature and classification of vitric and crystalline tuffs (after Pettijohn, 1975).

it often entraps air and may ride outward at very high speeds on this cushion. The material deposited from such eruptions usually are still very hot when they land. Fragments of still viscous glass usually weld together and flow under the weight of overlying tuff, forming a strong dense rock called welded tuff. Some such deposits are sufficiently thick and hot that portions of the glassy welded tuff recrystallize as the flow cools. These are called devitrified tuff.

The stratigraphy of tuffs and related volcanic ejecta is difficult to characterize. Because volcanic ejecta are deposited on land, original topographic variations affect lateral continuity of the deposits. Many tuffaceous deposits occur in tectonically active areas with complex depositional histories. In addition, the history of most rhyolitic volcanoes involves repeated building and collapse (caldera-formation) of volcanic edifices. Gradational changes in rock character relate to the cooling history of ash-flow, with a welded or devitrified core sandwiched between nonwelded upper and lower portions. The welded/devitrified zones often thin and disappear away from the source. These variations commonly occur over distances that are short compared to sedimentary facies transitions.

The stratigraphic sequence shown in Figure 5-4 is a schematic diagram of a compound ash-flow deposit interspersed with ash-fall layers. Note that the tops and bottoms of each flow are nonwelded, becoming better welded toward the center of each unit. Lithophysae (stone bubbles) are formed when gases are trapped in the cooling rock. The zones of vapor phase crystallization are formed by vapor and gases moving toward the top surface of the unit as it cools. The zones of reworked and/or bedded tuff indicate a hiatus after deposition of the sequence when the volcanic material is moved about by wind or water. Bedding is determined by particle size, the amount of sorting that has taken place, and whether the place of deposition is terrestrial or aquatic. The main constituents of reworked tuff are pumice and glass shards.

Tuff that is deposited in water or is at some time in the saturated zone undergoes fairly rapid alteration that is facilitated by the character of the loose tuff, i.e., the tuff is permeable, has a large surface area, and the glass particles are unstable. The alteration results in devitrification of the glass and formation of zeolites from the calcic, sodic, and potassic feldspar minerals. Alteration of volcanic tuff to zeolites is noted here because of their importance in retarding radionuclides that may migrate from a repository. The amount of alteration of tuffs is dependent upon the connected porosity in the tuffs and the availability of water. Zeolitization occurs at low temperatures (<200°C) and at

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Figure 5-4. Schematic diagram of internal structures within and relationships between tuff units.

low pressure (<300 MPa) in nonwelded vitric tuffs, which have a large porosity (Figure 5-5). Alteration in densely welded tuffs occurs in vugs and fractures. The main products of alteration of tuffs are zeolites and the smectite group of clay minerals.

The tuff repository is assumed to be located in the same area as Yucca Mountain, about 145 km north of Las Vegas, Nevada. The area contains numerous tuff deposits that lie within the Great Basin section of the Basin and Range physiographic province (refer to Figure 5-1). The section is located in the most arid part of this very arid province where the topography is characterized by a series of subparallel block-faulted mountain ranges separated by alluvial-filled intermontane desert basins. The Great Basin lies in the rain-shadow of the Sierra Nevada range and receives less than 25 cm of rain annually. It should be noted that the Great Basin is not technically a basin but instead is a series of internally drained basins that would be connected if there were enough surface runoff.

5.2 Tuff Stratigraphy at Yucca Mountain

This discussion of the regional stratigraphy of tuff is limited to southern Nevada because of the paucity of data for other tuffs. The stratigraphy of Yucca Mountain has been studied extensively for the purpose of developing a potential high-level radioactive waste repository in the unsaturated zone. The following discussion of unsaturated and saturated tuffs is taken freely from studies by Guzowski et al. (1983), Tien et al. (1985), and MacDougall et al. (1987a,b).

The regional stratigraphy of Yucca Mountain can be divided into four distinct units: Precambrian crystalline rocks, Late Precambrian and Paleozoic clastic rocks and carbonates, Tertiary volcanic rocks, and late Tertiary and Quaternary alluvium. Precambrian and Paleozoic rocks do not crop out nor have they been encountered in wells at the Yucca Mountain site, but observations of these rocks have been made at outcrops 15 km east of the Yucca Mountain and in a well 2.5 km outside of the study area. The Paleozoic rocks are made up predominantly of carbonates with some argillites and coarse clastics of Devonian and Mississippian age and may lie 3 km below Yucca Mountain. The presence of these carbonates is important in determining area hydrology.

The Tertiary volcanic rocks are the proposed repository host rocks at Yucca Mountain. The sequence of volcanics is a thick (>2000 m) series of rhyolitic tuffs, clastic lava flows, and flow breccias (Guzowski et al., 1983). Interspersed are reworked tuffaceous clastic rocks and ash-fall tuffs.

The youngest deposits are late Tertiary and Quaternary alluvial deposits consisting of silt, sand, and gravel derived from the ash flows and ash-fall tuffs.

Table 5-1 summarizes the Yucca Mountain stratigraphy. The sequence begins with the "older tuffs," which are comprised of up to 14 compound cooling units made up of moderately to densely welded ash flows and bedded/reworked tuffs with some ash-fall interbeds. The next unit, the Lithic Ridge Tuff, is an altered, quartz-poor tuff with plagioclase overlain by fractured flow breccias and bedded tuffs.

Overlying the flow breccias are the Crater Flat Tuff Formation which is, in turn, overlain by the Paintbrush Tuff Formation. The Crater Flat Tuff and the Paintbrush Tuff are made up of three and five members, respectively. The formations will be elevated to group status and the members will be given formation status in the near future (oral communication, C. Rautman, 1994).

5.3 Modeling the Tuff Repository

The diagram in Figure 5-6 illustrates the stratigraphy used in the conceptual model for this study. The left-hand side is a composite made from USW G-3 and USW G-4 well data and illustrates a profile of the stratigraphic members of the formations above the flow breccias and how weathering affects the resistive and nonresistive units. Densely welded units do not weather as readily as the reworked interbeds, which gives a rather distinct profile. The

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Figure 5-5. Alteration of tuff. The products of devitrification and zeolitization are called devitrified and zeolitized tuff, respectively. Glassy, densely welded tuffs and nonwelded tuffs that do not undergo alteration are called vitrophyres and vitric tuffs, respectively (after Guzowski et al., 1983).

Table 5-1. Stratigraphic Sequence at Tuff Repository Site

Age (millions of yr)*	Geologic Formations
11.3 to 12.6	Paintbrush Tuff Tiva Canyon Member Yucca Mountain Member Pah Canyon Member
12.1 to 13.3	Topopah Spring Member** Tuffaceous Beds of Calico Hills**
12.9 to 14.1	Crater Flat Tuff Prow Pass Member Bullfrog Member** Tram Member** (including Dacite Flow breccia) Flow Breccia Lithic Ridge Tuff** (Lithic-Rich Tuff) Older Tuffs

* Marvin et al., 1990.

** Potential subsurface facility levels.

5. Hypothetical Geologic Barrier

Figure 5-6. Stratigraphic column of Yucca Mountain tuffs. Thermal/hydrologic units are based on welding and/or porosity.

right-hand side of the figure delineates the hydrostratigraphic units, which are based on thermomechanical properties, as determined by amount of welding, vitrification, and zeolitization, and reworking of the tuffs, based on the well descriptions in Schenker et al. (1994). The central part of the figure is a composite plot of the porosity data, also from wells USW G-3 and USW G-4. Note the porosity changes corresponding to each hydrostratigraphic unit.

Table 5-2 describes the hydrostratigraphic units in the Yucca Mountain study area. Parameter values are described in Section 5.3.1 and listed in Tables 5-3 through 5-14.

5.3.1 Model Parameters for Tuff

This section lists the parameters used in the computational models discussed in Chapters 12 and 13. Although it is convenient in terms of organization to include the model parameters for the geologic barrier in this chapter, the reader may wish to defer examining them until he or she has read the discussion on the conceptual and mathematical models.

Hydrostratigraphic properties used in this performance assessment of a tuff repository are provided in Tables 5-3 to 5-14 for the hydrostratigraphic units shown in Table 5-2. The range of the parameters, the median value, and the source of the data are provided in these tables. The parameters shown in bold were sampled. Because the emphasis of the performance assessment was on the waste treatment options, only a few geologic barrier parameters were sampled. Several important parameters are described below.

Most of the parameter values were taken from a tuff parameter development report presented by Schenker et al., (1994). Published drillhole data from 23 wells were used to categorize each unit in terms of its physical characteristics (welding) and its hydrologic characteristics. The thermomechanical and hydrologic parameters compiled for fractures and matrix (when applicable) are welding, porosity, permeability, fracture density, compressibility, diffusion coefficient, residual saturation, specific heat, thermal expansion coefficient, thermal conductivity, dispersivity, and tortuosity. An overview of the parameter development can also be found in Wilson et al. (1994).

Physical Parameters. Important physical parameters are matrix porosity, bulk density, saturated hydraulic conductivity, water retention, residual saturation, and bulk combined conductivities.

Matrix Porosity. Over 1200 matrix porosity measurements have been made on the hydrostratigraphic units at Yucca Mountain, making this one of the most comprehensive data sets for the site. The composite porosity measurements show how the hydrostratigraphic units in Figure 5-6 correlate to the units picked from the lithologic logs of well USW G-3 and USW G-4. The mean porosity for the welded units ranges from 0.06 to 0.29 and for the unwelded units from 0.26 to 0.42. The reworked bedded tuffs of the Pah Canyon and Yucca Mountain Members of the Paintbrush Tuff have the highest porosities (up to 0.65).

Matrix Bulk Density. Because bulk density measurements of the tuffs at Yucca Mountain form another large data set with over 2600 measurements, the basic statistics were calculated directly. The expected values for the 11 hydrostratigraphic units range from 1714 kg/m³ for the bedded, reworked Pah Canyon to 2366 kg/m³ for the welded Tiva Canyon.

Matrix Saturated Hydraulic Conductivity. Hydraulic conductivity data were assigned to their respective hydro-stratigraphic unit based on the model stratigraphy. More than 250 values were analyzed. Mean values for the 11 units range from 10⁻¹¹ m/s in the lower Topopah Spring thin welded unit (TSwv) to 10⁻⁶ m/s for the Pah Canyon (PTn).

Water Retention. Water retention data are available only for the upper 10 of the 11 hydrostratigraphic units. Mean values for the 10 units range from 0.018 1/m for the welded Prow Pass Member to 0.2458 1/m for the Pah Canyon Member.

Table 5-2. Descriptions of Eleven Hydrogeologic Units Used in the INEL 1994 PA*

Unit Number	Hydrogeologic Unit	Predominate Mineral Form	Description**
1	TCw	Devitrified	The portion of the Tiva Canyon member of the Paintbrush Tuff Formation that consists of moderately to densely welded, devitrified (minerals converted to crystalline forms) ash flows (Material 1, see Table 5-4).
2	PTn	Devitrified	Nonwelded to partially welded, vitric and locally devitrified tuffs belonging to the lowermost Tiva Canyon Member, Yucca Mountain Member, Pah Canyon Member and uppermost Topopah Spring Member of the Paintbrush Tuff Formation; also includes airfall tuffs, "bedded tuffs," and intercalated reworked tuffaceous sediments. The Yucca Mountain and Pah Canyon Members are locally welded to the north of the repository region (Material 2, see Table 5-5).
3	TSw	Devitrified	Moderately to densely welded, devitrified ash-flow tuffs (including the upper vitrophyre) belonging to the portion of the Topopah Spring Member of the Paintbrush Tuff Formation (Material 3, see Table 5-6).
4	TSwv	Vitric	Densely welded basal vitrophyre belonging to the Topopah Spring Member of the Paintbrush Tuff Formation (Material 4, see Table 5-7).
5	CHnv	Vitric	Nonwelded to partially welded, vitric (minerals in glass) and argillaceous ash-flow, bedded, and reworked tuffs belonging to a lowermost part of the Topopah Spring Member of the Paintbrush Tuff Formation and the tuffaceous beds of Calico Hills (Material 5, see Table 5-8).
6	CHnz	Zeolitic	Similar to CHnv, but consisting of the zeolitized portions (hydrous aluminosilicate minerals that exchange ions of Na, Ca, Ba, Sr, and K easily) of tuffaceous beds of Calico Hills and the nonwelded portion of the Prow Pass member of the Crater Flat Tuff Formation (Material 6, see Table 5-9).
7	PPw	Devitrified	Partially to moderately welded, devitrified and locally zeolitic ash-flow tuffs belonging to the Prow Pass Member of the Crater Flat Tuff Formation (Material 7, see Table 5-10).
8	CFUn	Zeolitic	Nonwelded to partially welded tuffs belonging to lower portion of Prow Pass Member and upper portion of Bullfrog Member of Crater Flat Tuff Formation (Material 8, see Table 5-11).
9	BFw	Devitrified	Moderately to densely welded, devitrified ash-flow tuffs belonging to the Bullfrog Member of the Crater Flat Tuff Formation (Material 7, see Table 5-10).
10	CFMn	Zeolitic	Nonwelded to partially welded, argillic, zeolitic, and devitrified ash-flow tuffs and minor "bedded tuffs" belonging to the lower portions of the Bullfrog Member and upper portion of the Tram Member of the Crater Flat Tuff Formation. Hydrologic flow and transport properties are assumed to be identical to CFUn (Material 9, see Table 5-12).
11	TRw	Devitrified	Moderately to densely welded, devitrified ash-flow tuffs belonging to the Tram Member of the Crater Flat Tuff Formation (Material 10, see Table 5-13).

* Primarily based on degree of welding, i.e., porosity.

** The hydrologic unit descriptions are general and may cross stratigraphic boundaries.

Table 5-3. Tiva Canyon Welded Tuff Thermal/Mechanical Hydrologic Parameter (Material 1)

Record No.	Parameter	Parameter Description	Median	Range		Units	Type	Sources In:
7302	DNSBLK	Bulk Density	2.402e+003	1.410e+003	2.530e+003	kg/m ³	BETA	Wilson et al., 1994
7300	BLKKGAS	Combined bulk saturated hydraulic conductivities	-4.598	-6.636	-3.936	m/s	BETA	Wilson et al., 1994
8032	COMPRES	Compressibility of rock	3.000e-011			Pa ⁻¹	CONSTANT	Guzowski et al., 1983
7311	FRACSPAC	Fracture spacing	1.091e-002	0	13.444	m	BETA	Wilson et al., 1994
7312	HYCNDSAM	Hydraulic conductivity, saturated in matrix	-11.012	-12.610	-8.320	m/s	BETA	Wilson et al., 1994
7315	POROSITY	Matrix porosity	6.875e-002	3.300e-002	0.450	none	BETA	Wilson et al., 1994
7316	RESISAT	Residual saturation	9.082e-004	0	1.000	m/s	BETA	Wilson et al., 1994
7318	SPCHET	Specific heat welded	728.000			J/kg*K	CONSTANT	Nimick and Connolly, 1991
9147	THRMCOND	Thermal conductivity (dry)	1.510			W/m*K	CONSTANT	YMP RIB, 1989
9148	THRMCONW	Thermal conductivity (wet)	1.630			W/m*K	CONSTANT	YMP RIB, 1989
9161	THRMEX	Thermal expansion non-welded	8.200			1/K	CONSTANT	YMP RIB, 1989
7323	TORTFRAC	Tortuosity in fractures	1.000			none	CONSTANT	Analyst decision
7324	TORTMATR	Tortuosity in matrix	10.000			none	CONSTANT	Analyst decision
7328	VGALPHA	Van Genuchten alpha coefficient (air-entry)	-2.066	-3.523	-0.874	l/m	BETA	Wilson et al., 1994
7329	VGBETA	Van Genuchten beta coefficient (sat/desat)	0.199	0.130	0.319	none	BETA	Wilson et al., 1994

Table 5-4. Paintbrush Non-Welded Tuff Thermal/Mechanical Hydrologic Parameter (Material 2)

Record No.	Parameter	Parameter Description	Median	Range	Units	Type	Sources In:
9149	THRMCOND	Thermal conductivity (dry)	0.610		W/m ² *K	CONSTANT	YMP RIB, 1989
9150	THRMCONW	Thermal conductivity (wet)	1.000		W/m ² *K	CONSTANT	YMP RIB, 1989
6917	THRMEX	Thermal expansion non-welded	2.900		1/K	CONSTANT	YMP RIB, 1989
6902	DNSBLK	Bulk Density	1.706e+003	850.000	kg/m ³	BETA	Wilson et al., 1994
6900	BLKGAS	Combined bulk saturated hydraulic conductivities	-5.282	-6.751	m/s	BETA	Wilson et al., 1994
9119	COMPRES	Compressibility of rock	1.000e-010		Pa ⁻¹	CONSTANT	Guzowski et al., 1983
6910	HYCNDSAM	Hydraulic conductivity, saturated in matrix	-6.854	-11.540	m/s	BETA	Wilson et al., 1994
6912	POROSITY	Matrix porosity	0.425	0.132	none	BETA	Wilson et al., 1994
6913	RESISAT	Residual saturation	9.036e-002	0	m/s	BETA	Wilson et al., 1994
6915	SPCHET	Specific heat welded	422.000		J/kg*K	CONSTANT	Nimick and Connolly, 1991
6920	TORTFRAC	Tortuosity in fractures	1.000		none	CONSTANT	Analyst decision
6921	TORTMATR	Tortuosity in matrix	10.000		none	CONSTANT	Analyst decision
6924	VGALPHA	Van Genuchten alpha coefficient (air-entry)	-1.298	-1.983	l/m	BETA	Wilson et al., 1994
6925	VGBETA	Van Genuchten beta coefficient (sat/desat)	0.292	7.400e-002	none	BETA	Wilson et al., 1994
6909	FRACSPAC	fracture spacing	3.778e-002	1.000e-003	m	BETA	Wilson et al., 1994
6912	POROSITY	porosity	0.425	0.132	none	BETA	Wilson et al., 1994

Table 5-5. Topopah Spring Welded Composite Tuff Thermal/Mechanical Hydrologic Parameter (Material 3)

Record No.	Parameter	Parameter Description	Median	Range	Units	Type	Sources In:
7702	DNSBLK	Bulk density	2.258e+003	1.686e+003 2.830e+003	kg/m ³	BETA	Wilson et al., 1994
7700	BLKKGAS	Combined bulk saturated hydraulic conductivities	-4.766	-5.319 -3.936	m/s	BETA	Wilson et al., 1994
8034	COMPRES	Compressibility of rock	5.000e-010		Pa ⁻¹	CONSTANT	Guzowski et al., 1983
8012	FRACSPAC	Fracture spacing	1.448e-002	0 19.878	m	BETA	Wilson et al., 1994
7707	HYCNDSAM	Hydraulic conductivity, saturated in matrix	-10.760	-12.520 -8.280	m/s	BETA	Wilson et al., 1994
7709	POROSITY	Matrix porosity	0.134	4.000e-003 0.480	none	BETA	Wilson et al., 1994
7710	RESISAT	Residual saturation	2.117e-002	0 1.000	m/s	BETA	Wilson et al., 1994
7712	SPCHET	Specific heat welded	840.000		J/kg*K	CONSTANT	Nimick and Connolly, 1991
9151	THRMCOND	Thermal conductivity (dry)	2.100		W/m*K	CONSTANT	YMP RIB, 1989
9152	THRMCONW	Thermal conductivity (wet)	2.100		W/m*K	CONSTANT	YMP RIB, 1989
9209	THRMEX	Thermal expansion non-welded	8.200		1/K	CONSTANT	YMP RIB, 1989
8008	TORTFRAC	Tortuosity in fractures	1.000		none	CONSTANT	Analyst decision
8007	TORTMATR	Tortuosity in matrix	10.000		none	CONSTANT	Analyst decision
7717	VGALPHA	Van Genuchten alpha coefficient (air-entry)	-1.953	-2.678 -0.372	l/m	BETA	Wilson et al., 1994
7718	VGBETA	Van Genuchten beta coefficient (sat/desat)	0.209	6.300e-002 0.729	none	BETA	Wilson et al., 1994

Table 5-6. Topopah Spring Vitrophyre Tuff Thermal/Mechanical Hydrologic Parameter (Material 4)

Record No.	Parameter	Parameter Description	Median	Range	Units	Type	Sources In:
7601	DNSBLK	Bulk density	2.318e+003	2.090e+003 2.400e+003	kg/m ³	BETA	Wilson et al., 1994
5000	BLKKGAS	Combined bulk saturated hydraulic conductivities	-4.774	-5.319 -3.936	m/s	BETA	Wilson et al., 1994
8035	COMPRES	Compressibility of rock	3.000e-011		Pa ⁻¹	CONSTANT	Guzowski et al., 1983
7610	FRACSPAC	Fracture spacing	1.737e-002	0 23.854	m	BETA	Wilson et al., 1994
7611	HYCNDSAM	Hydraulic conductivity, saturated in matrix	-11.019	-11.820 -10.160	m/s	BETA	Wilson et al., 1994
7614	POROSITY	Matrix porosity	5.457e-002	1.400e-002 0.177	none	BETA	Wilson et al., 1994
7615	RESISAT	Residual saturation	4.104e-002	0 1.000	m/s	BETA	Wilson et al., 1994
7617	SPCHET	Specific heat welded	948.000		J/kg*K	CONSTANT	Nimick and Connolly, 1991
9153	THRMCOND	Thermal conductivity (dry)	1.260		W/m*K	CONSTANT	YMP RIB, 1989
9154	THRMCONW	Thermal conductivity (wet)	1.280		W/m*K	CONSTANT	YMP RIB, 1989
9162	THRMEX	Thermal expansion non-welded	10.600		1/K	CONSTANT	YMP RIB, 1989
8006	TORTFRAC	Tortuosity in fractures	1.000		none	CONSTANT	Analyst decision
7622	TORTMATR	Tortuosity in matrix	10.000		none	CONSTANT	Analyst decision
7625	VGALPHA	Van Genuchten alpha coefficient (air-entry)	-2.511	-3.699 -2.114	l/m	BETA	Wilson et al., 1994
7626	VGBETA	Van Genuchten beta coefficient (sat/dsat)	0.301	0.139 0.651	none	BETA	Wilson et al., 1994

Table 5-7. Calico Hills Non-Welded Vitric/Vitrified Tuff Thermal/Mechanical Hydrologic Parameter (Material 5)

Record No.	Parameter	Parameter Description	Median	Range		Units	Type	Sources In:
6402	DNSBLK	Bulk density	1.816e+003	1.050e+003	3.020e+003	kg/m ³	BETA	Wilson et al., 1994
6400	BLKKGAS	Combined bulk saturated hydraulic conductivities	-5.286	-6.751	-3.627	m/s	BETA	Wilson et al., 1994
8036	COMPRES	Compressibility of rock	7.000e-010			Pa ⁻¹	CONSTANT	Guzowski et al., 1983
6411	FRACSPAC	Fracture spacing	3.134e-002	0	42.465	m	BETA	Wilson et al., 1994
6412	HYCND SAM	Hydraulic conductivity, saturated in matrix	-9.003	-11.290	-6.540	m/s	BETA	Wilson et al., 1994
6415	POROSITY	Matrix porosity	0.336	9.700e-002	0.510	none	BETA	Wilson et al., 1994
6417	RESISAT	Residual saturation	3.657e-002	0	1.000	m/s	BETA	Wilson et al., 1994
6419	SPCHET	Specific heat welded	488.000			J/kg*K	CONSTANT	Nimick and Connolly, 1991
9155	THRMCOND	Thermal conductivity (dry)	0.840			W/m*K	CONSTANT	YMP RIB, 1989
9156	THRMCONW	Thermal conductivity (wet)	1.240			W/m*K	CONSTANT	YMP RIB, 1989
6421	THRMEX	Thermal expansion non-welded	2.900			1/K	CONSTANT	YMP RIB, 1989
6424	TORTFRAC	Tortuosity in fractures	1.000			none	CONSTANT	Analyst decision
6425	TORTMATR	Tortuosity in matrix	10.000			none	CONSTANT	Analyst decision
6428	VGALPHA	Van Genuchten alpha coefficient (air-entry)	-1.750	-2.268	-0.426	l/m	BETA	Wilson et al., 1994
6429	VGBETA	Van Genuchten beta coefficient (sat/desat)	0.318	9.700e-002	0.995	none	BETA	Wilson et al., 1994

Table 5-8. Calico Hills Non-Welded Zeolitic Tuff Thermal/Mechanical Hydrologic Parameter (Material 6)

Record No.	Parameter	Parameter Description	Median	Range		Units	Type	Sources In:
6503	DNSBLK	Bulk density	1.743e+003	1.300e+003	2.230e+003	kg/m ³	BETA	Wilson et al., 1994
6500	BLKKGAS	Combined bulk saturated hydraulic conductivities	-5.890	-7.360	-4.870	m/s	BETA	Wilson et al., 1994
8037	COMPRES	Compressibility of rock	1.000e-009			Pa ⁻¹	CONSTANT	Guzowski et al., 1983
6512	FRACSPAC	Fracture spacing	3.988e-002	0	54.046	m	BETA	Wilson et al., 1994
6513	HYCND SAM	Hydraulic conductivity, saturated in matrix	-10.754	-13.630	-8.500	m/s	BETA	Wilson et al., 1994
6516	POROSITY	Matrix porosity	0.306	0.141	0.470	none	BETA	Wilson et al., 1994
6517	RESISAT	Residual saturation	4.163e-002	0	1.000	m/s	BETA	Wilson et al., 1994
6519	SPCHET	Specific heat welded	526.000			J/kg*K	CONSTANT	Nimick and Connolly, 1991
9157	THRMCOND	Thermal conductivity (dry)	0.560			W/m*K	CONSTANT	YMP RIB, 1989
9158	THRMCONW	Thermal conductivity (wet)	1.350			W/m*K	CONSTANT	YMP RIB, 1989
6521	THRMEX	Thermal expansion non-welded	9.300			1/K	CONSTANT	YMP RIB, 1989
6524	TORTFRAC	Tortuosity in fractures	1.000			none	CONSTANT	Analyst decision
8005	TORTMATR	Tortuosity in matrix	10.000			none	CONSTANT	Analyst decision
6527	VGALPHA	Van Genuchten alpha coefficient (air-entry)	-2.320	-3.398	-0.628	l/m	BETA	Wilson et al., 1994
6528	VGBETA	Van Genuchten beta coefficient (sat/desat)	0.194	7.300e-002	0.772	none	BETA	Wilson et al., 1994

Table 5-9. Prow Pass Welded Tuff Thermal/Mechanical Hydrologic Parameter (Material 7)

Record No.	Parameter	Parameter Description	Median	Range		Units	Type	Sources In:
7102	DNSBLK	Bulk density	1.934e+003	1.440e+003	3.120e+003	kg/m ³	BETA	Wilson et al., 1994
7100	BLKKGAS	Combined bulk saturated hydraulic conductivities	-5.799	-8.045	-2.282	m/s	BETA	Wilson et al., 1994
8038	COMPRES	Compressibility of rock	1.000e-009			Pa ⁻¹	CONSTANT	Guzowski et al., 1983
7111	FRACSPAC	Fracture spacing	5.249e-002	1.000e-003	61.469	m	BETA	Wilson et al., 1994
7112	HYCNSAM	Hydraulic conductivity, saturated in matrix	-8.861	-11.020	-8.050	m/s	BETA	Wilson et al., 1994
7115	POROSITY	Matrix porosity	0.296	0.101	0.430	none	BETA	Wilson et al., 1994
7116	RESISAT	Residual saturation	6.219e-002	0	1.000	m/s	BETA	Wilson et al., 1994
7118	SPCHET	Specific heat welded	728.000			J/kg*K	CONSTANT	Nimick and Connolly, 1991
9159	THRMCOND	Thermal conductivity (dry)	1.350			W/m*K	CONSTANT	YMP RIB, 1989
9160	THRMCONW	Thermal conductivity (wet)	2.000			W/m*K	CONSTANT	YMP RIB, 1989
9163	THRMEX	Thermal expansion non-welded	8.200			1/K	CONSTANT	YMP RIB, 1989
7123	TORTFRAC	Tortuosity in fractures	1.000			none	CONSTANT	Analyst decision
7124	TORTMATR	Tortuosity in matrix	10.000			none	CONSTANT	Analyst decision
7127	VGALPHA	Van Genuchten alpha coefficient (air-entry)	-1.781	-2.071	-1.463	l/m	BETA	Wilson et al., 1994
7128	VGBETA	Van Genuchten beta coefficient (sat/desat)	0.757	0.388	1.230	none	BETA	Wilson et al., 1994

Table 5-10. Bull Frog Welded Tuff Thermal/Mechanical Hydrologic Parameter (Material 8)

Record No.	Parameter	Parameter Description	Median	Range		Units	Type	Sources In:
6202	DNSBLK	Bulk density	2.282e+003	1.800e+003	2.510e+003	kg/m ³	BETA	Wilson et al., 1994
6200	BLKKGAS	Combined bulk saturated hydraulic conductivities	-5.435	-7.819	-4.604	m/s	BETA	Wilson et al., 1994
8039	COMPRES	Compressibility of rock	5.000e-010			Pa ⁻¹	CONSTANT	Guzowski et al., 1983
6211	FRACSPAC	Fracture spacing	1.448e-002	0	19.878	m	BETA	Wilson et al., 1994
6212	HYCND SAM	Hydraulic conductivity, saturated in matrix	-9.190	-10.710	-9.030	m/s	BETA	Wilson et al., 1994
6215	POROSITY	Matrix porosity	0.181	5.800e-002	0.231	none	BETA	Wilson et al., 1994
6216	RESISAT	Residual saturation	2.117e-002	0	1.000	m/s	BETA	Wilson et al., 1994
6218	SPCHET	Specific heat welded	858.300	795.500	921.100	J/kg*K	UNIFORM	Nimick and Connolly, 1991
6223	TORTFRAC	Tortuosity in fractures	1.000			none	CONSTANT	Analyst decision
6224	TORTMATR	Tortuosity in matrix	10.000			none	CONSTANT	Analyst decision
6226	VGALPHA	Van Genuchten alpha coefficient (air-entry)	-1.953	-2.678	-0.372	l/m	BETA	Wilson et al., 1994
6227	VGBETA	Van Genuchten beta coefficient (sat/desat)	0.209	6.300e-002	0.729	none	BETA	Wilson et al., 1994

Table 5-11. Bull Frog Non-Welded Tuff Thermal/Mechanical Hydrologic Parameter (Material 9)

Record No.	Parameter	Parameter Description	Median	Range		Units	Type	Sources In:
6102	DNSBLK	Bulk density	2.037e+003	1.600e+003	2.320e+003	kg/m ³	BETA	Wilson et al., 1994
6100	BLKKGAS	Combined bulk saturated hydraulic conductivities	-7.013	-8.524	-6.033	m/s	BETA	Wilson et al., 1994
8040	COMPRES	Compressibility of rock	7.000e-010			Pa ⁻¹	CONSTANT	Guzowski et al., 1983
6111	FRACSPAC	Fracture spacing	5.249e-002	1.000e-003	61.469	m	BETA	Wilson et al., 1994
6112	HYCND SAM	Hydraulic conductivity, saturated in matrix	-8.561	-9.640	-7.870	m/s	BETA	Wilson et al., 1994
6115	POROSITY	Matrix porosity	0.257	0.174	0.380	none	BETA	Wilson et al., 1994
6116	RESISAT	Residual saturation	5.639e-002	0	1.000	m/s	BETA	Wilson et al., 1994
6118	SPCHET	Specific heat welded	1.256e+003	795.500	1.717e+003	J/kg*K	UNIFORM	Nimick and Connolly, 1991
6123	TORTFRAC	Tortuosity in fractures	1.000			none	CONSTANT	Analyst decision
6124	TORTMATR	Tortuosity in matrix	10.000			none	CONSTANT	Analyst decision
6127	VGALPHA	Van Genuchten alpha coefficient (air-entry)	-1.772	-2.009	-1.449	l/m	BETA	Wilson et al., 1994
6128	VGBETA	Van Genuchten beta coefficient (sat/desat)	0.447	0.309	0.679	none	BETA	Wilson et al., 1994

Table 5-12. Tram Member Welded Tuff Thermal/Mechanical Hydrologic Parameter (Material 10)

Record No.	Parameter	Parameter Description	Median	Range		Units	Type	Sources In:
7502	DNSBLK	Bulk density	2.193e+003	1.800e+003	2.470e+003	kg/m ³	BETA	Wilson et al., 1994
7500	BLKKGAS	Combined bulk saturated hydraulic conductivities	-5.783	-7.562	-4.589	m/s	BETA	Wilson et al., 1994
8041	COMPRES	Compressibility of rock	5.000e-010			Pa ⁻¹	CONSTANT	Guzowski et al., 1983
7505	HYCNDSAM	Hydraulic conductivity, saturated in matrix	-8.967	-10.640	-8.240	m/s	BETA	Wilson et al., 1994
7507	POROSITY	Matrix porosity	0.200	1.800e-002	0.280	none	BETA	Wilson et al., 1994
7508	SPCHET	Specific heat welded	858.300	795.500	921.100	J/kg*K	UNIFORM	Nimick and Connolly, 1991
7513	TORTFRAC	Tortuosity in fractures	1.000			none	CONSTANT	Analyst decision
7514	TORTMATR	Tortuosity in matrix	10.000			none	CONSTANT	Analyst decision

Table 5-13. Fracture Properties

Record No.	Parameter	Parameter Description	Median	Range		Units	Type	Sources In:
7995	RESISAT	Residual saturation	4.00e-002			m/s	CONSTANT	YMP RIB, 1989
7994	VGBETA	Van Genuchten beta coefficient (sat/ desat)	3.00e+000	1.80e+000	4.20e+000	none	UNIFORM	Wilson et al., 1994

Table 5-14. Elicited Sorption Coefficient (Kd) Distributions (m³/kg) for Elements as a Function of Rock Type (Modified from Wilson et al., 1994)

Element	Parameter	Expected	Minimum Values	Maximum Values	Coefficient of Value	Units	Type
Actinium	KDD	1.05e+000	1.00e-001	2.00e+000	---	m ³ /kg	UNIFORM
	KDV	3.96e-001	1.00e-001	1.00e+000	0.200	m ³ /kg	BETA
	KDZ	5.50e-001	1.00e-001	1.00e+000	---	m ³ /kg	UNIFORM
	KDFE	3.00e+000	1.00e+000	5.00e+000	---	m ³ /kg	UNIFORM
Americium	KDD	1.05e+000	1.00e-001	2.00e+000	---	m ³ /kg	UNIFORM
	KDV	3.96e-001	1.00e-001	1.00e+000	0.200	m ³ /kg	BETA
	KDZ	5.50e-001	1.00e-001	1.00e+000	---	m ³ /kg	UNIFORM
	KDFE	3.00e+000	1.00e+000	5.00e+000	---	m ³ /kg	UNIFORM
Carbon	KDD	0	0	0	---	m ³ /kg	CONSTANT
	KDV	0	0	0	---	m ³ /kg	CONSTANT
	KDZ	0	0	0	---	m ³ /kg	CONSTANT
	KDFE	0	0	0	---	m ³ /kg	CONSTANT
	KDI	4.60e+001	4.60e+001	4.60e+001	---	none	CONSTANT
	KDS	-4.75e-001	-4.75e-001	-4.75e-001	---	none	CONSTANT
Chlorine	KDD	0	0	0	---	m ³ /kg	CONSTANT
	KDV	0	0	0	---	m ³ /kg	CONSTANT
	KDZ	0	0	0	---	m ³ /kg	CONSTANT
	KDFE	0	0	0	---	m ³ /kg	CONSTANT
Cesium	KDD	1.50e-001	1.00e-001	2.00e-001	---	m ³ /kg	UNIFORM
	KDV	1.50e-001	1.00e-001	2.00e-001	---	m ³ /kg	UNIFORM
	KDZ	1.75e+000	5.00e-001	3.00e+000	---	m ³ /kg	UNIFORM
	KDFE	5.98e-002	0	2.50e-001	1.000	m ³ /kg	BETA
Iodine	KDD	0	0	0	---	m ³ /kg	CONSTANT
	KDV	0	0	0	---	m ³ /kg	CONSTANT
	KDZ	0	0	0	---	m ³ /kg	CONSTANT
	KDFE	0	0	0	---	m ³ /kg	CONSTANT
Niobium	KDD	1.05e+000	1.00e-001	2.00e+000	---	m ³ /kg	UNIFORM
	KDV	3.96e-001	1.00e-001	1.00e+000	0.200	m ³ /kg	BETA
	KDZ	5.50e-001	1.00e-001	1.00e+000	---	m ³ /kg	UNIFORM
	KDFE	3.00e+000	1.00e+000	5.00e+000	---	m ³ /kg	UNIFORM
Nickel	KDD	2.50e-001	0	5.00e-001	0.330	m ³ /kg	BETA
	KDV	2.50e-001	0	5.00e-001	0.330	m ³ /kg	BETA
	KDZ	2.50e-001	0	5.00e-001	0.330	m ³ /kg	BETA

Table 5-14. Elicited Sorption Coefficient (Kd) Distributions (m³/kg) for Elements as a Function of Rock Type (Modified from Wilson et al., 1994) (Continued)

Element	Parameter	Expected	Minimum Values	Maximum Values	Coefficient of Value	Units	Type
	KDFE	2.50e-001	2.50e-001	2.50e-001	---	m ³ /kg	CONSTANT
Neptunium	KDD	1.38e-003	0	5.00e-002	1.000	m ³ /kg	BETA
	KDV	3.45e-004	0	1.25e-002	1.000	m ³ /kg	BETA
	KDZ	2.76e-003	0	1.00e-001	1.000	m ³ /kg	BETA
	KDFE	7.50e-001	5.00e-001	1.00e+000	---	m ³ /kg	UNIFORM
Protactinium	KDD	1.38e-003	0	5.00e-002	1.000	m ³ /kg	BETA
	KDV	6.94e-004	0	1.25e-001	1.000	m ³ /kg	BETA
	KDZ	2.76e-003	0	1.00e-001	1.000	m ³ /kg	BETA
	KDFE	7.50e-001	5.00e-001	1.00e+000	---	m ³ /kg	UNIFORM
Lead	KDD	2.50e-001	0	5.00e-001	---	m ³ /kg	UNIFORM
	KDV	3.00e-001	1.00e-001	5.00e-001	---	m ³ /kg	UNIFORM
	KDZ	3.00e-001	1.00e-001	5.00e-001	---	m ³ /kg	UNIFORM
	KDFE	5.50e-001	1.00e-001	1.00e+000	---	m ³ /kg	UNIFORM
Plutonium	KDD	9.75e-002	5.00e-002	2.00e-001	0.250	m ³ /kg	BETA
	KDV	9.75e-002	5.00e-002	2.00e-001	0.250	m ³ /kg	BETA
	KDZ	3.91e-002	3.00e-002	7.00e-002	0.150	m ³ /kg	BETA
	KDFE	3.00e+000	1.00e+000	5.00e+000	---	m ³ /kg	UNIFORM
Radium	KDD	3.00e-001	1.00e-001	5.00e-001	---	m ³ /kg	UNIFORM
	KDV	3.00e-001	1.00e-001	5.00e-001	---	m ³ /kg	UNIFORM
	KDZ	3.00e+000	1.00e+000	5.00e+000	---	m ³ /kg	UNIFORM
	KDFE	2.07e-002	0	7.50e-001	1.000	m ³ /kg	BETA
Selenium	KDD	2.50e-003	0	5.00e-003	---	m ³ /kg	UNIFORM
	KDV	2.00e-003	0	4.00e-003	---	m ³ /kg	UNIFORM
	KDZ	9.61e-003	5.00e-003	2.00e-002	0.300	m ³ /kg	BETA
	KDFE	5.50e-001	1.00e-001	1.00e+000	---	m ³ /kg	UNIFORM
Sumarium	KDD	1.05e+000	1.00e-001	2.00e+000	---	m ³ /kg	UNIFORM
	KDV	3.96e-001	1.00e-001	1.00e+000	0.200	m ³ /kg	BETA
	KDZ	5.50e-001	1.00e-001	1.00e+000	---	m ³ /kg	UNIFORM
	KDFE	3.00e+000	1.00e+000	5.00e+000	---	m ³ /kg	UNIFORM
Tin	KDD	1.10e-001	2.00e-002	2.00e-001	---	m ³ /kg	UNIFORM
	KDV	1.10e-001	2.00e-002	2.00e-001	---	m ³ /kg	UNIFORM
	KDZ	2.00e-001	1.00e-001	3.00e-001	---	m ³ /kg	UNIFORM

Table 5-14. Elicited Sorption Coefficient (Kd) Distributions (m³/kg) for Elements as a Function of Rock Type (Modified from Wilson et al., 1994) (Continued)

Element	Parameter	Expected	Minimum Values	Maximum Values	Coefficient of Value	Units	Type
Strontium	KDFE	2.50e+000	0	5.00e+000	---	m ³ /kg	UNIFORM
	KDD	1.05e-001	1.00e-002	2.00e-001	---	m ³ /kg	UNIFORM
	KDV	3.50e-002	2.00e-002	5.00e-002	---	m ³ /kg	UNIFORM
	KDZ	1.00e+001	1.00e+001	1.00e+001	---	m ³ /kg	CONSTANT
	KDFE	3.50e-002	2.00e-002	5.00e-002	---	m ³ /kg	UNIFORM
Technetium	KDD	0	0	0	---	m ³ /kg	CONSTANT
	KDV	0	0	0	---	m ³ /kg	CONSTANT
	KDZ	0	0	0	---	m ³ /kg	CONSTANT
	KDFE	0	0	0	---	m ³ /kg	CONSTANT
Thorium	KDD	1.05e+000	1.00e-001	2.00e+000	---	m ³ /kg	UNIFORM
	KDV	3.96e-001	1.00e-001	1.00e+000	0.200	m ³ /kg	BETA
	KDZ	5.50e-001	1.00e-001	1.00e+000	---	m ³ /kg	UNIFORM
	KDFE	3.00e+000	1.00e+000	5.00e+000	---	m ³ /kg	UNIFORM
Uranium	KDD	2.50e-003	0	5.00e-003	---	m ³ /kg	UNIFORM
	KDV	2.00e-003	0	4.00e-003	---	m ³ /kg	UNIFORM
	KDZ	9.61e-003	5.00e-003	2.00e-002	0.300	m ³ /kg	BETA
	KDFE	5.50e-001	1.00e-001	1.00e+000	---	m ³ /kg	UNIFORM
Zirconium	KDD	1.05e+000	1.00e-001	2.00e+000	---	m ³ /kg	UNIFORM
	KDV	3.96e-001	1.00e-001	1.00e+000	0.200	m ³ /kg	BETA
	KDZ	5.50e-001	1.00e-001	1.00e+000	---	m ³ /kg	UNIFORM
	KDFE	3.00e+000	1.00e+000	5.00e+000	---	m ³ /kg	UNIFORM

Matrix Residual Saturation. Mean values for residual saturation range from 0.0212 for the Tiva Canyon Member to 0.1540 for the Pah Canyon.

Bulk Combined Conductivities. The values of the combined conductivities come from bulk saturated conductivity, barometric gas conductivity, and analog values. The analog values were obtained by matching characteristics of hydrostratigraphic units and using known values for the untested units. Log₁₀ values of the conductivities range from -7.0625 to -4.7424.

Hydrologic Parameters of Fractures. Fractures or partings of rock allow faster movement of groundwater, and so their orientation, frequency, and morphology are important for developing a conceptual model of groundwater flow in tuff. Fractures in tuffs occur when compressional, tensional, and shear stresses from shrinkage by drying or cooling, tectonic activity, erosional unloading, or weathering act on the rock mass. If displacement of the rock is not evident, the fractures are called joints; if displacement is evident, the fractures are called faults. Evidence of movement in fractured tuffs are offset of fragments, brecciation, and slickensides. Parameters for fractures can be found in Tables 5-3 through 5-13.

Fracture frequency seems to be strongly influenced by the degree of welding of the hydrostratigraphic unit. An average for apparent fracture frequencies per 10 m based on welding are 25.6 for densely welded tuffs of the Tiva Canyon, 4.4 for moderately welded to nonwelded tuffs of the Tiva Canyon, Yucca Mountain, Pah Canyon, and Topopah Spring, 13.3 for the densely welded Topopah Spring, 0.9 for the tuffaceous beds of the Calico Hills, and 2.9 for the moderately welded deeper tuffs at well G-4 (Spengler et al., 1984). Similar conclusions about units with high fracture frequency were made from other well data and observations in the area (Spengler et al., 1979; Spengler et al., 1981). Many fractures, e.g., 88% in one well (Spengler et al., 1981) show evidence of at least partial coatings by secondary minerals. In about 40% of these fractures, most of which are in the tuffaceous beds of the Calico Hills or deeper, the void space was completely filled with minerals.

Joints in the Tiva Canyon have nearly random dip angles from 0° to 90° caused by cooling (high angle) and release of overburden pressure (low angle). The lower Topopah Spring and the tuffaceous beds of the Calico Hills have high angle joints probably from tensional forces (Spengler et al., 1979). Fractures apparently are not connected across the units. Flow in the unsaturated, highly fractured, densely welded units is rapid in the vertical direction; flow in the unsaturated, tuffaceous and reworked tuffs is horizontal. The matrix of the densely welded tuffs has a low effective porosity, and the matrix of the nonwelded and reworked tuffs has higher porosities.

Fracture properties that can be measured are frequency (number/meter) and orientation (dip angle). The fracture parameters required for this study are spacing (2B), porosity (ϕ_f), air-entry parameter (α_{VGf}), aperture (b_f) and permeability (k_f). Fracture frequency and orientation are measured values from four representative drill holes that bound the tuff repository (Arnold et al., 1995). The relationship used to derive the remaining fracture parameters is explained in the next section.

Fracture Frequency (F_f). Fracture frequencies were compiled from downhole data reported in original USGS Open File Reports by Spengler et al. (1981, 1984, 1979) and Scott and Castellanos (1984) for drill holes USW G-1, USW G-4, UE-25#1, and USW GU-3, respectively. The data, which were presented as number of fractures per 3 m interval, were converted to number of fractures per meter, grouped according to hydrostratigraphy, and analyzed. The coefficients of variation for the fracture frequency are near one. Wilson et al. (1994) assumed that because, by definition, an exponential distribution has a coefficient of variation of 1.0, all the fracture distributions can be represented by beta function probability distributions that approximate exponential distributions with a minimum of zero and a maximum of infinity. The maximum was set at 30 times the mean to approximate an exponential probability distribution function by a beta function, resulting in a beta distribution close to the desired exponential. Note that as a result, the exponents for fracture frequency are the same for all hydrostratigraphic units.

Fracture Orientation (θ_f). Fracture orientation parameters were derived for hydrostratigraphic units 1, 2, 3, and 5 from the wells listed above and served as analogs for the remaining units (4, 6, 7, 8, and 9). Unit 10 was not considered (Schenker et al., 1994; Wilson et al., 1994).

Fracture Spacing (s). Fracture spacing was computed from the fracture frequency and fracture orientation using the method established for the other parameters. A set of 100 values was computed and the statistics derived for the units modeled (Arnold et al., 1995).

Modeling Parameters Used for Fractures. The fracture network porosity (ϕ_f), permeability (k_f), and the parameter used to express the characteristic wetting and drying curve (α_{VG}), are required in the models discussed in Chapters 12 and 13. However, these three parameters are not measured directly. Rather they are derived from other rock properties that are more easily measured, such as values of fracture frequency (N), fracture orientation (θ_f), bulk hydraulic conductivity (k_b), and matrix hydraulic conductivity (k_m), which were described above. The following sections describe how these four measured values are used to generate the three necessary modeling parameters.

Fracture Porosity. The data reduction model used to arrive at the fracture porosity (ϕ_f) was the parallel plate model (although we recognize the theory is now outdated). Snow (1968) derived an expression relating the permeability of the fracture network to the fracture aperture and spacing,

$$k_f = \frac{b^3}{12s}, \quad (5-1)$$

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where, k_f is the fracture permeability, b is the aperture, and s is the fracture spacing. For determining the fracture porosity, k_f was assumed to be equal to the bulk permeability, k_b . Setting $k_f = k_b$, and solving Equation 5-1 for the fracture aperture, we have

$$b = \sqrt[3]{12sk_b} \quad (5-2)$$

The fracture spacing was obtained from the fracture orientation and fracture frequency as

$$s = \frac{\cos(\phi_f)}{N} \quad (5-3)$$

The bulk permeability, k_b , was obtained from the bulk hydraulic conductivity (K_b) using the relationship

$$k_b = K_b \mu / \rho g \quad (5-4)$$

where $\mu = 1.12 \times 10^{-3}$ Ns/m², $\rho = 1000$ kg/m³, and $g = 9.81$ m/s². From the fracture aperture, b , and fracture spacing, s , the fracture porosity of the parallel plate model, ϕ_f , is computed simply as,

$$\phi_f = \frac{b}{s} \quad (5-5)$$

Fracture Permeability. The permeability of the fracture network is evaluated assuming that the bulk permeability can be expressed as a parallel flow system in terms of the matrix and fracture permeability, k_m and k_f , and the matrix and fracture cross-sectional area, A_m and A_f

$$k_b = \frac{A_m k_m + A_f k_f}{A_m + A_f} \quad (5-6)$$

Recognizing that, $\phi_f = A_f / (A_f + A_m)$ and $1 - \phi_f = A_m / (A_f + A_m)$, the fracture continuum permeability is

$$k_f = \frac{k_b - (1 - \phi_f) k_m}{\phi_f} \quad (5-7)$$

Water Retention Air Entry Parameter (α_{VG}). Corey (1986) shows that the entry pressure P_o , between two parallel plates can be computed from the aperture b_f , interfacial surface tension σ , and the contact angle, θ

$$P_o = \frac{2\sigma \cos \theta}{b_f} \quad (5-8)$$

For this study, the contact angle (θ) is assumed to be zero, and the interfacial surface tension (σ) equal to 0.072 kg/s² for an air/water system.

The air entry parameter in the van Genuchten equation for the characteristic wetting and drying curve is the inverse of the pressurehead,

$$\alpha_{VG} = \frac{\rho g}{P_o} \quad (5-9)$$

5.3.2 Modeling Assumptions

General

- Fluid (gas and liquid) flow obeys Darcy's law.
- Host formation is unsaturated (see Chapter 12).
- Host formation is underlain by saturated zone (see Chapter 12).
- Other strata are assumed not to affect the repository.
- Bedding planes are horizontal.
- Constant layer thickness.
- Fixed water table elevation.
- Homogeneous layers.

Paintbrush Tuff

- Repository is in a thick, densely devitrified tuff (Topopah Spring Member).
- Formation is of high porosity and low permeability.
- Formation is unsaturated.

Calico Hills Nonwelded Zeolitic Layer

- Layer formation is saturated.
- Aquifer is hydrologically unconfined with no vertical leakage.
- Fluctuations in aquifer flow caused by climate changes are considered.
- Dual porosity model without chemical retardation adequately describes radionuclide transport in aquifer.

Table 5-15 lists the sampled parameters for the unsaturated zone flow modeling. Table 5-16 lists the layers modeled and the sampled parameters that are assigned. For example, layer TCw (welded Tiva Canyon) has the same parameter values as TSw (welded Topopah Spring).

Table 5-15. Unsaturated Zone Geologic Sampling Parameters

Variable Name	Description	Assigned Unit
VGBETA	matrix van Genuchten " β "	(TSw, CHnv, PPw)
BULKKGAS	bulk hydraulic conductivity	(TSw, CHnv, PPw)
FRACSPAC	fracture spacing	(TSw, CHnv, PPw)
HYCNDSAM	matrix hydraulic conductivity	(TSw, CHnv, PPw)

Table 5-16. Analog Units

Layer	VGBETA	BULKKGAS	FRACSPAC	HYCNDSAM
TCw	TSw	TSw	TSw	TSw
PTn	CHnv	CHnv	CHnv	CHnv
TSw	TSw	TSw	TSw	TSw
TSv	mean	TSw	TSw	mean
CHnv	CHnv	CHnv	CHnv	CHnv
CHnz	TSw	CHnv	CHnv	TSw
PPw	PPw	PPw	PPw	PPw

5.4 Percolation Variation from Climate Changes

(R.P. Rechar and M.L. Wilson)

As mentioned at the beginning of this chapter, the function of the geologic barrier is to isolate the waste from the accessible environment. However, it must also provide a reasonably stable chemical and physical environment for the nuclear waste. Although agents (either events or processes) acting upon the geologic barrier could enhance its behavior, the primary emphasis in deciding what can happen to the geologic barrier (scenario development) is on debilitating agents. One such agent identified in Chapter 7, "Scenario Development," is climate change that causes an increase in water percolating through the repository. Although climate change is not part of the geologic barrier, it is an agent that acts directly upon it and thus is discussed in this chapter. Table 5-17 lists parameters for agents acting upon the disposal system.

Throughout the following discussion, infiltration is defined as the passage of water through the soil surface *into* the soil and percolation is the movement of water *through* the soil.

5.4.1 Influence of Climate Change

Climate change indirectly influences the geologic barrier and its ability to isolate the waste. Although not modeled in this performance assessment, the complete process is iterative and complex: Climate directly influences precipitation, which affects infiltration into the soil. The infiltration affects vegetation on the surface and percolation through the soil, both of which strongly influence infiltration through feedback effects.

The 1994 PA focuses on how the geologic barrier is influenced by potential variations in infiltration as the result of climate change, and the ability of the geologic barrier to moderate these changes. No attempt is made to predict the future climate of the surface area. The record of past climate is used to guide estimates of future infiltration, as described below.

5.4.2 Infiltration Variation Model

The model uses a sine function for the potential variation in infiltration. Minimum and maximum infiltration rates are determined for both wet and dry climates.

Sine Function for Modeling Infiltration Variation. Fairly persuasive evidence has been documented that Pleistocene climate underwent a periodic progression of changes associated with glacial cycles (Imbrie and Imbrie, 1979; Imbrie, 1985). The extremes of these cycle are glacial (or pluvial) and interglacial conditions. Studies of pack-rat middens (e.g., Spaulding, 1985), ostracods (e.g., Forester, 1987), lake levels (e.g., Benson et al., 1990), and water-table levels (e.g., Paces et al., 1993, and Marshall et al., 1993), indicate that, in the southwestern United States as a whole, the glacial periods were typically "wet," whereas the interglacials were typically "dry." The present climate is an interglacial, dry climate.

A sine function was selected to model the potential variation in infiltration (Figure 5-7).

$$I = I_{\min} + \left(\frac{I_{\max} - I_{\min}}{2} \right) \left[1 - \cos \left(\frac{2\pi t}{T} \right) \right] \quad (5-10)$$

where I is the infiltration at time t , $I_{\min}$ and $I_{\max}$ are the dry- and wet-climate infiltration rates, and T is the period of the sine function. This function is used, not to predict future infiltration, but to approximate the variability in infiltration that may occur. The extent to which unprecedented climatic changes caused by human-induced changes in the composition of the earth's atmosphere may invalidate this assumption is not certain. Many models that evaluate the influence of increased gases from the greenhouse effect on climate change predict that changes will be no more extensive

Table 5-17. Agents Acting on Tuff Disposal System

Record No.	Parameter	Parameter Description	Median	Range		Units	Type	Sources In:
6650	CYCLEPER	Climatic cycle period	1.00e+005	4.00e+004	1.60e+005	years	UNIFORM	Wilson et al., 1994
9071	LAMBDAG	Drilling intrusion into Tuff Repository	4.75e-018	0	9.51e-018	m ⁻² s ⁻¹	UNIFORM	EPA, 1985, Appendix C
6653	PPTINFOC	Infiltration focus	5.50e+000	1.00e+000	1.00e+001	none	UNIFORM	See text, Chapter 5
6652	PPTINFMX	Maximum infiltration in cycle	1.00e+001	1.00e+000	1.90e+001	mm/yr	UNIFORM	Wilson et al., 1994
6651	PPTINFMN	Minimum infiltration in cycle	5.00e-001	0	1.00e+000	mm/yr	UNIFORM	Wilson et al., 1994
9210	DIAMMOD	Modern or current diameter	2.65e-001	5.08e-002	6.10e-001	m	DELTA	Craft et al., 1962

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Figure 5-7. Sine function representing annual infiltration fluctuations in next 100,000 yr.

sive than those of the Pleistocene, although rates of change will likely be greater (e.g., Mitchell, 1989; Houghton et al., 1990).

Period of Wet and Dry Climates. The major glacial cycles are about 100,000 years long on average and appear to correlate with changes in the amount of solar radiation that reaches the Earth, known as the Milankovitch insolation cycles (Imbrie and Imbrie, 1979). These changes are caused by the eccentricity in the Earth's orbit around the Sun (a 100,000-yr period), the tilt of the Earth's axis (a 41,000-yr period), and the precession of the Earth's axis (19,000- and 23,000-yr periods). Winograd et al. (1988) suggest a slightly different timescale, one not aligned with the Milankovitch insolation cycles; however, Imbrie et al. (1993) argue that the difference is not significant. Prior to 400,000 years ago, the primary period appears to have been 41,000 years rather than 100,000 years. A 41,000-yr period actually aligns better with the insolation cycle; there is no simple insolation explanation for the current 100,000-yr dominant period. We cannot be sure if the 100,000-yr period will persist for another cycle, but it presently appears to be a reasonable working hypothesis. For this study, a uniform distribution of periods was used, uniform from 40,000 yr to 160,000 yr (mean of 100,000 yr).

The breakdown of climate variation into regular cycles is, of course, an idealization; there is actually considerable variation from one cycle to the next and within cycles. Boulton and Payne (1992) summarized a number of predictions of future climate cycles and noted that major cold phases between 15,000 and 35,000 years in the future and between 54,000 and 70,000 years in the future were common to all of them. Some of the models also predicted a cold phase 5000 to 8000 years from now. In addition, there is evidence from Greenland ice cores that there may be significant climate variations on much shorter time scales (GRIP, 1993).

Minimum and Maximum Infiltration Rates. Given that wet and dry climates have affected Yucca Mountain, it is necessary to specify likely infiltration rates. For the infiltration rate during dry periods, a uniform distribution from 0 to 1 mm/yr (mean of 0.5 mm/yr) is used; for the infiltration rate during wet periods, a uniform distribution from 1 to 19 mm/yr (mean of 10 mm/yr) is used.

Dry Climate. The infiltration distribution for the dry climate is believed to be representative of current, interglacial conditions. Estimated percolation rates range between 10^{-7} and 10^{-2} mm/yr for Yucca Mountain (see, for example, Gauthier, 1993; Weeks and Wilson, 1984; Montazer and Wilson, 1984; and Flint et al., 1993). These estimates are for single-phase flow through the matrix, although indirectly they could include flow through fractures if matrix and fracture flow are coupled.

Estimates of recharge to the saturated zone (which would include matrix, fracture, and vapor flow) have been made based on gross water balance—precipitation minus estimated runoff and evapotranspiration. Nevada State hydrologists have devised a method—the “Maxey-Eakin” method—for estimating recharge based on elevation and precipitation (Maxey and Eakin, 1949; Eakin et al., 1951). Table 5-18 contains a summary of recharge for the Ash Meadows groundwater system based on the Maxey-Eakin method (Rush, 1971). The summit of Yucca Mountain is at an elevation somewhat higher than 1500 m. Additional elevations are included in the table because with climate change, a region can effectively act as if it were a different elevation.

Table 5-18. Recharge for Various Precipitation Zones in the Ash Meadows Groundwater System as Predicted by the Maxey-Eakin Method (summarized from Rush, 1971).

Precipitation Zone (m)	Precipitation Range (mm/yr)	Recharge as Percentage of Precipitation	Infiltration Range (mm/yr)
>2400	>500	25	>120
2100-2400	400-500	15	60-80
1800-2100	300-400	7	20-30
1500-1800	200-300	3	6-9
<1500	<200	Minor	---

Studies show that for the present climate at the Yucca Mountain region, there is negligible recharge and the numbers above must be upper limits to what is negligible (Rush, 1971; Rice, 1984; Flint et al., 1993). Long and Childs (1993) devised a fairly elaborate model of precipitation and infiltration for the EPRI performance assessment (McGuire et al., 1992) and came up with an infiltration estimate of 0.9 ± 0.5 mm/yr.

A uniform probability distribution for infiltration was chosen because it is a simple functional form, gives equal weight to all infiltrations, and requires only one parameter to be defined. The mean value of 0.5 mm/yr was chosen because it was thought that a very low value (near zero) was likely, but that some weight to the possibility of higher values such as those listed above was warranted.

Wet Climate. The wet-climate infiltration distribution represents conditions at a “full glacial maximum”— nominally the wettest period of a glacial cycle. Estimates of infiltration during a full glacial maximum come from modeling and field investigation, but data are sparse and extrapolations from the data are speculative. Models have predicted increases in infiltration from current conditions to full glacial maximum from 0.02 mm/yr (Flint et al., 1993) to 2.4 ± 1.4 mm/yr (Long and Childs, 1993).

As an alternative to modeling, infiltration during a glacial maximum can be estimated by treating areas near Yucca Mountain, such as Pahute Mesa and Rainier Mesa, as possible analogs of Yucca Mountain during a global ice-

age climate. As shown in Table 5-7, Rush (1971) estimated a recharge of about 7% of precipitation from elevations in the 1800- to 2100-m range. (Rainier Mesa is at about 2200-m elevation, and Pahute Mesa is a little lower). It has been estimated from actual observations that parts of Rainier Mesa have a recharge of about 8% of precipitation, or 24 mm/yr (Wang et al., 1993).

For the 1994 PA, the wet-climate infiltration is described using a uniform distribution with a mean of 10 mm/yr. The lower limit is set to 1 mm/yr to assure a wet-climate infiltration higher than the dry climate infiltration. This distribution is based on Spaulding's (1985) estimate of 40% higher precipitation during a glacial maximum. This increase would result in an annual precipitation of about 240 mm/yr ($170 \text{ mm/yr} \times 1.4$). Using Table 5-15, this value correlates with an effective elevation increase of several hundred meters at Yucca Mountain, and infiltration would be expected to be approximately 3% of this value, or 7 mm/yr ($240 \text{ mm/yr} \times 0.03$). Evapotranspiration and other environmental effects are taken into account in the Maxey-Eakin method, and thus, changes in vegetation, temperature, cloudiness, the amount of sunlight reaching the ground, etc., are accounted for.

The uniform distribution with a mean of 10 mm/yr allows for the possibility of even greater infiltrations at Yucca Mountain during a full glacial maximum. The distribution includes infiltrations as high as 19 mm/yr. We feel that it is reasonable to include such high infiltration values for three reasons: (1) field investigations show a possible correspondence in vegetation growth between Yucca Mountain at a full glacial maximum and areas 1200 m higher under present conditions. Using Table 5-18, an elevation that is 1200 m higher than Yucca Mountain—2700 m—would have an infiltration of over 120 mm/yr. This effective elevation is even higher (and wetter) than Rainier Mesa; (2) based on an analysis of fossil ostracod species from deposits laid down approximately 15,000 years ago in southern Nevada, Forester and Smith (1992) predict an annual mean temperature of 9°C (as opposed to 17°C presently) and an annual precipitation value greater than the present value for Rainier Mesa; and (3) Swift (1992) concluded that the evidence from a number of sources suggest that the annual precipitation was a factor of 2 higher at the last glacial maximum in southern New Mexico. At Yucca Mountain, twice the present-day precipitation would be approximately 340 mm/yr. Using Table 5-15, this value correlates with an effective elevation of between 1800 and 2100 m, and a recharge of 7% of percolation; 7% of $2 \times 170 \text{ mm/yr}$ is about 24 mm/yr—coincidentally, the same as parts of Rainier Mesa. However if the jet stream was directly over southern New Mexico, but south of Nevada, then the increase in precipitation in southern New Mexico might be an overestimate of the increase in precipitation in southern Nevada.

5.4.3 Percolation in Simple PA

Infiltration, movement of water *into* the soil, and percolation, movement of water *through* the soil, are closely related because infiltration cannot continue unless percolation removes water from the surface soil. This interaction is particularly important for the one-dimensional model used in the Simple PA.

The relationship between near-surface infiltration and deep percolation is assumed to be the same in the Complex PA (Chapter 13), i.e., all water that makes it past the zone of evapotranspiration flows through 2D model fractures all the way down to the water table. Past modeling that has been done using the 2D composite-porosity model (Ross, 1990; Prindle and Hopkins, 1990) has found significant lateral flow in the nonwelded Paintbrush (unit 2—PTn—in Table 5-2), above the repository, when infiltration is high. In fact, Ross showed that this unit might act as a capillary barrier because its pores are smaller than the fracture apertures in the Topopah Spring welded unit (unit 3—TSw). The capillary-barrier hypothesis is that water would avoid the TSw fractures, preferring to flow laterally in the PTn matrix. If this is the case, the TSw matrix might flow at capacity under wet conditions, but the fractures would not flow. For the Simple PA's one-dimensional composite-porosity model (Chapter 13), however, with its assumption of one-dimensional flow with no outlet for large infiltration, such an assumption is not reasonable. The implication is that the saturated conductivity of the TSw matrix (K_{sm}) is the maximum attainable percolation rate. Thus, the distribution of values for K_{sm} is important.

In TSPA-1993 (Wilson et al., 1994), this argument was used to justify a decrease in percolation in the one-dimensional flow and transport model when the infiltration rate exceeded the conductivity of the TSw hydrologic modeling layer. For the 1994 PA, however, it was decided to simplify further and assume that percolation equals infiltration, for

the Simple PA as well as the Complex PA. This assumption should be conservative in relation to the TSPA-1993 assumption of reduced percolation.

Because steady-state water flow was used for the Simple PA calculations, the infiltration function given in Equation 5-1 was averaged over the 10,000-yr period of the calculations, and the flow calculated using the average infiltration value:

$$I_{ave} = \frac{I_{min} + I_{max}}{2} - \frac{1}{2\pi} \frac{T}{t} \left(\frac{I_{max} - I_{min}}{2} \right) \sin (2\pi t / T) \quad (5-11)$$

where $t = 10,000$ yr. A histogram of the I_{ave} values used in the calculations is given in Chapter 13 (Figure 13-11).

6. Repository Design

J. S. Rath

Although the geological environment surrounding the waste can be viewed as the ultimate barrier protecting the accessible environment, the engineered barrier can offer additional protection. Components of the engineered barrier may include (not all are necessary):

1. Durable waste forms that are resistant to alteration (Chapter 4).
2. Containers that serve to protect the waste from groundwater (Chapter 4).
3. Subsurface facility layout that is constructed to accomplish particular objectives such as prevention of undue host rock disturbances from waste decay heat, diminution of groundwater movement by avoiding discovered fracture zones, or orientation of drifts perpendicular to regional groundwater gradients.
4. Waste parcel placement that diminishes, for example, either temperature increases in the host rock,* groundwater movement, or neutron interaction between containers.
5. Specially placed backfill in the shafts, drifts, rooms, and directly around the waste parcel, to limit groundwater movement and chemically retard radionuclide transport.

The latter three items (subsurface facility layout, emplacement of waste parcels, and backfill) are components of repository design. This chapter provides dimensions of the subsurface facility layout, details about the waste emplacement schemes and their effect on repository design, and a discussion of backfill.

6.1 Subsurface Facilities

The disposal region of the repository has been sized to accommodate 12,060 MTHM of spent fuel or equivalent high-level waste based on the number of waste parcels from INEL, Savannah River, Hanford, and West Valley.

The hypothetical repository modeled in the 1994 PA is loosely patterned after the proposed repository layout for the Yucca Mountain Project. The hypothetical repository is placed 306 m below the surface (top of alluvium to repository floor) and is a room and pillar configuration for both vertical and horizontal emplacement, with the entire repository consisting of rooms ("tunnels") (Figures 6-1 and 6-2). The rooms are surrounded by access drifts, 7.62 m in width for perimeter ventilation. An access drift for people and machinery runs along the length of one side of the repository (Figures 6-1 and 6-2), and leads to ramps that connect to the surface. A tunnel boring machine is assumed for excavation of the rooms and drifts and is the preferred mining scheme for the Yucca Mountain Project (TRW, 1993a).

General repository dimensions are provided in Table 6-1; these dimensions correspond to the layout when waste types are disposed of as a group with the INEL high-level waste as a glass-ceramic waste form (Complex PA). For the Simple PA, where waste parcels are studied individually, the number of waste parcels was increased or decreased to maintain the same total heat output and so the number of rooms and repository area change. The design of the repository is governed by the total waste volume (12,060 MTHM) and the emplacement of the waste parcels, as discussed below. Figures 6-1 and 6-2 provides dimensions for the repository layout for horizontal and vertical emplacements, respectively.

6.2 Emplacement of Waste Parcels

For this performance assessment, two orientations for placement of waste parcel are considered: horizontal emplacement within the rooms and vertical emplacement in boreholes in disposal rooms floors. The technical baseline design for the Yucca Mountain Project as of February, 1994, is horizontal emplacement, in which a limited num-

* Some designs incorporate enhancement of temperatures to keep moisture from containers for a longer period of time.

6. Repository Design

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Figure 6-1. Layout of waste disposal rooms and access drifts for hypothetical repository in tuff for horizontal emplacement scheme.

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Figure 6-2. Layout of waste disposal rooms and access drifts for hypothetical repository in tuff for vertical emplacement scheme.

Table 6-1. Dimensions of Subsurface Facilities for Disposal of Mixed Waste in Complex PA*

Region	Dimensions	
	Horizontal Emplacement	Vertical Emplacement
Waste disposal rooms	Length: 426 m Diameter: 4.3 m Total: 59 rooms	Length: 426 m Width: 7.62 m Total: 38 rooms
Pillars	Length: 426 m Width: 4.3 m	Length: 426 m Width: 7.60 m
Access drifts	Width: 7.62 m	Width: 7.62 m
Repository (total)	$2.56 \times 10^5 \text{ m}^2$	$2.98 \times 10^5 \text{ m}^2$
Waste disposal area (excavated)	$1.08 \times 10^5 \text{ m}^2$	$1.27 \times 10^5 \text{ m}^2$
Extraction ratio	42%	42%

* These dimensions assume that all the DOE spent fuel and high-level waste will be disposed of as a group with the INEL calcine high-level waste as a glass-ceramic waste form.

ber of large containers would be transported by rail both to and within the repository. The proposed container for the horizontal emplacement is a 125-ton MPC, which would be parked in the rooms for disposal. (See Chapter 4 for a discussion of the container.) Vertical emplacement corresponds to the orientation modeled in the 1993 PA for INEL and to early conceptual designs for waste emplacement in the U.S. and other countries (e.g., SCP, 1988). Vertical emplacement uses 25-ton LWT canisters and DOE standard canisters (see also Chapter 4).

With both orientations, three factors potentially affect the spacing of waste parcels within the rooms and the distance between rooms: (1) thermal limits placed on the waste form and/or adjacent host rock, (2) ability to bore closely spaced boreholes and/or tunnel closely spaced rooms, and (3) potential for neutron interaction between containers, which would enhance the possibility of a critical condition.

Table 6-2 provides a listing of the number of containers required to dispose of the spent fuel and high-level waste. (See also Chapter 4 for additional information about waste volume and types.)

6.2.1 Horizontal Emplacement for Complex PA

For horizontal emplacement, the 1994 PA had a thermal design goal of reaching as high an areal power density as possible with the relatively cool DOE spent nuclear fuel and high-level waste. The goal was based on continuing studies by the Yucca Mountain Project to actively consider a high areal power density to determine whether any desirable effects are encountered, such as whether the host rock dries out for hundreds of years.[†] Figure 6-3 shows the area for calculating the design-basis areal power density.[‡]

[†] The benefit of high temperatures in an unsaturated repository is a hypothesis that is under active consideration for horizontal emplacement by the Yucca Mountain Project. The 1994 PA adopted the hypothesis to be consistent with the current thinking of the Yucca Mountain Project; however, the 1994 PA did not use a high power areal density for the vertical emplacement.

[‡] The design-basis areal power density is calculated using an entire room and half the width of the pillars and access drifts around the room to define the area. However, because of the regular shape of the disposal area, this value is equivalent to a local areal power density, which is the area around a single container and half the distance to adjacent containers.

Table 6-2. Quantity of Containers and Heat Rates for the Spent Nuclear Fuel and High-Level Waste Modeled in the 1994 Performance Assessment

Waste Type	Waste Parcel ID	Quantity for Complex PA	Container Type	Length of Container (m)	Power (W)
Horizontal					
Graphite	101	83	SF-MPC ^a	5.29	170
N-Reactor	102	59	SF-MPC	5.29	1630
Shippingport	103	295	SF-MPC	5.29	2020
ATR (HEU)	104	53	SF-MPC	5.29	871
PWR (LEU)	105	36	SF-MPC	5.59	2180
INEL calcine, glass ceramic	106	2037	DHLW-MPC ^b	3.70	30
Savannah River	107	1321	DHLW-MPC	3.70	1312
Hanford	108	49	DHLW-MPC	3.70	1564
West Valley	109	69	DHLW-MPC	3.70	588
INEL calcine, borosilicate glass	110	7249	DHLW-MPC	3.70	8.0
INEL calcine, loose powder	111	1737	DHLW-MPC	3.70	34
Vertical					
Graphite	201	560	LWT ^c	4.50	25.4
N-Reactor	202	394	LWT	4.50	244
Shippingport	203	1540	LWT	4.50	337
ATR (HEU)	204	233	LWT	4.50	597
PWR (LEU)	205	252	LWT	4.50	312
INEL calcine, glass ceramic	206	8147	DOE standard	3.00	7.5
Savannah River	207	5283	DOE standard	3.00	328
Hanford	208	1960	DOE standard	3.00	391
West Valley	209	276	DOE standard	3.00	147
INEL calcine, borosilicate glass	210	28994	DOE standard	3.0	2.0
INEL calcine, loose powder	211	6945	DOE standard	3.0	8.52

^a SF-MPC – 125-ton multi-purpose canister for spent nuclear fuel

^b DHLW-MPC – 125-ton multi-purpose canister for defense high-level waste

^c LWT – 25-ton legal weight truck container

- L_R = Length of Active Waste Disposal Room
- O_S = Distance of Waste from Access Drift
- D_W = Room Width
- D_S = Pillar Width
- $A_{APDDR} = (L_R + 2O_S + 3 \cdot D_W) \cdot (D_S + D_W)$

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Figure 6-3. Area for calculating the design-basis areal power density (APD).

Areal power densities are achieved by controlling the spacing among nearest-neighbor waste parcels. The waste parcels have a heat output at the time of emplacement that depends on the burnup and decay of the spent fuel. (The heat output from high-level waste containers is also considered but is relatively low.) The accumulated heat from all the parcels in the repository creates repository-scale thermal effects (e.g., heating and dryout) in the surrounding rock. The amount of heat produced varies with time and is a function of the time that the radioisotopes have decayed (fuel "age") and the original irradiation of the fuel in the nuclear reactors (fuel "burnup"). The heat rates for the spent fuel and waste modeled in the 1994 PA are shown in Table 6-2.

Waste Parcel Spacing. To produce the highest areal power density possible for horizontal emplacement, the MPCs are modeled as remaining on the underground rail transportation and placed end-to-end without spacing (Figure 6-4). Neutron interaction, which is a criticality consideration, was shown to be minimal because of the large amount of material present in the lids of the MPCs. (These and other criticality considerations are presented in Chapter 10.)

Two other thermal limits were considered in the horizontal emplacement design for the Complex PA, in which a mix of waste was evaluated: (1) a maximum centerline temperature in a waste parcel to prevent excessive failures of fuel cladding and (2) a host rock/waste parcel interface temperature below 200°C to prevent undesirable thermal stresses around the room. The maximum centerline temperature was 350°C for most fuels and 200°C for the aluminum-clad ATR fuel, which represents the highly enriched fuel. A third thermal limit, which was not designed into the repository but is evaluated in the results, is maintaining a temperature below 115°C at the interface of two hydrologic modeling units Tswv and Chn (see Chapter 5). This limit was originally proposed in conceptual designs of the Yucca Mountain repository to prevent alteration of zeolites in the hydrologic modeling unit, Chnz, which is directly below Chn; alteration of zeolites may reduce their ability to absorb radionuclides (MacDougall et al., 1987b). However, neither the importance of Chnz to the disposal system performance nor the alteration of the zeolites from a temperature pulse has been confirmed, and so its potential for influencing radionuclide sorption was not considered in repository design.

To maintain the power density at the same level as the Complex PA for individual fuels, the Simple PA, which evaluated only one waste type at a time, adjusted the quantity (MTHM) of the fuel, the total power output of the fuel, and the spacing of the containers. The Simple PA did not consider the two thermal limits; the centerline temperature limit was exceeded by 20°C for the ATR spent fuel, and the limit for the host-rock/waste parcel interface was exceeded by 80°C for the Hanford borosilicate glass waste.

Room Spacing. Room diameter for the horizontal emplacement scheme is 4.3 m (Figure 6-1) and is drawn from the baseline technical design for the Yucca Mountain Project (TRW, 1993a, p. 5-44). Rooms were spaced with the constraint that the pillar that separates the rooms be no less than the width of the room diameter, and thus a 4.3-m room spacing was modeled. Although the ability to tunnel rooms this close together was not examined in detail, it appeared to be plausible.

Enclosed Area. The combination of end-to-end spacing of the MPCs and the room spacing of 4.3 m resulted in a design-basis areal power density of 23.5 W/m² in the year 2030 (see also Appendix E). This value represents the maximum areal power density that could be realistically obtained with the assumed mix of DOE spent nuclear fuel and high-level waste. The resulting enclosed area of the disposal region is 0.288 km² with an extraction ratio of 42%. Table 6-3 provides repository design parameters.

6.2.2 Vertical Emplacement for Complex PA

The design goal of the 1994 PA for vertical emplacement was to achieve an areal power density of 14.1 W/m² (57 kW/acre) to be consistent with an early conceptual design goal for the Yucca Mountain Project. Achieving an areal power density higher than 14.1 W/m² for a vertical emplacement scheme is difficult because of construction constraints; neither boreholes nor rooms can be placed closer together than the spacing modeled. Note that in the 1993 PA, the design-basis areal power densities for waste disposal group 1 (minimal treatment) for the salt and granite disposal systems were 5.3 W/m² and 4.6 W/m², respectively.

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Figure 6-4. Waste disposal room and multi-purpose canister (MPC) emplacement cart for horizontal, indrift emplacement. The MPC is first placed in two disposal overpack containers and then transported by rail to the disposal room.

Table 6-3. Repository Design Geometry Parameters for Disposal of Mixed Waste in the Complex PA

Parameter	Horizontal	Vertical
Design-Basis Areal Power Density	23.6 W/m ²	14.0 W/m ²
Length of waste disposal room for design ^a	1.7001×10^4 m	1.6185×10^4 m
Average power of waste in MPC	786.06 W	184.92 W
Pillar width	4.3 m	7.60 m
Waste disposal room		
Diameter	4.3 m	7.62 m
Length of room	426 m	426 m
Length available for waste disposal	422 m	422 m
Offset ^b	2 m	2 m
Number of waste disposal rooms	59	38
Number of waste parcels per room	75	489
Total capacity of waste parcels in repository	4425	19071
Repository		
Length	542.1 m	631.66 m
Width (parallel to drifts)	471.72 m	471.72 m
Area	2.5576×10^5 m ²	2.9797×10^5 m ²
Disposal region, area excavated	1.0808×10^5 m ²	1.266×10^5 m ²
Extraction ratio ^c	42.26%	42.48%
Repository power density ^d	13.474 W/m ²	11.572 W/m ²

^a One waste emplacement drift is used for calculations for design-basis areal power density.
^b Offset is the portion at either end of the room that is not filled with waste.
^c Extraction ratio equals excavated area divided by repository area.
^d Repository power density equals total power of all the waste divided by repository area and is different from the design-basis areal power density.

Waste Parcel Spacing. For spacing of waste parcels in the vertical emplacement scheme, the geometric constraints considered were rock stability, construction requirements, and maximum number of waste parcels per disposal room. According to Wilson et al. (1994), rock stability requires a minimum of 2.29-m center-to-center spacing. A thermal constraint was a maximum temperature of 100°C at the host rock/waste parcel interface to reduce vaporization of groundwater. (This same constraint was considered in the 1993 PA.) The generally low temperatures produced by the DOE spent nuclear fuel and high-level waste permitted a minimum spacing of 2.6 m (8.5 ft) center-to-center in a compact hexagonal pattern in the room (Figure 6-5).

The minimum spacing for actual construction is a 2.6-m center-to-center hexagonal spacing, which was also recently adopted as the spacing to maximize thermal loading (Cowell et al., 1994). The spacing required to limit neutron interaction between canisters fell below this range (see Appendix B).

Room Spacing. Room width for the vertical emplacement scheme is 7.62 m (Figure 6-5), which is based on the disposal design used in TSPA-1993 (Wilson et al., 1994). The areal power density equation was used to calculate room spacing:

$$\text{Design-Basis APD} = \frac{P}{(L_R + 2O_s + 3D_w)(D_s + D_w)}$$

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Figure 6-5. Waste disposal room for vertical, borehole emplacement in tuff repository.

where

- P = total power
- L_R = length of a single waste disposal room containing all waste parcels for a given disposal orientation (i.e., vertical or horizontal)
- O_s = Offset of waste from edge of access drift
- D_w = Room width
- D_s = Pillar width

Spacing of the waste disposal rooms for the 1994 PA was found by rearranging the areal power density equation and decomposing the area into length and width parameters (see also Appendix E). Once the spacing value was known, then values for the length of the waste emplacement room, the number of waste parcels per room, and the number of rooms were computed. More information about how the room spacings were calculated is provided in Appendix E, Scoping Calculations. Table 6-3 provides the parameters used for the repository design.

Waste Parcel Boreholes. Two different-sized boreholes are required to accommodate the spent fuel and high-level waste containers for vertical emplacement. The LWT containers are 0.75-m in diameter, and the DOE standard containers are 0.63-m in diameter. These dimensions include a 2.54-cm air gap between each waste parcel and the host rock (see Section 6.2.3, Backfill).

Each borehole is plugged with a steel plug for diminishing gamma rays. The borehole plug is the diameter of the borehole it is sealing (i.e., either 0.75 m or 0.63 m) and is 1 m long. A typical waste parcel borehole plug is shown in Figure 6-5.

Enclosed Area. The combination of the 2.6-m spacing of the boreholes and an areal power density of 14.1 W/m^2 in the year 2030 resulted in a 7.5-m spacing between rooms (slightly smaller than the width of the room itself). The resulting enclosed area of the disposal region is 0.247 km^2 , which is somewhat smaller than the horizontal emplacement scheme; however, the extraction ratio of 42% is the same.

6.2.3 Differences Between Emplacement Schemes

Differences between the horizontal and vertical emplacements for the Complex PA are listed in Table 6-4. Differences in repository areas for the Simple PA are listed in Table 6-5.

6.3 Backfill for Emplacement Schemes

As used in this report, backfill is the material that seals the excavated openings of the repository. Special categories of backfill include (a) seals for providing immediate sealing of access drifts and ramps and (b) backfill-buffer,** which is placed directly around the waste parcel. In the 1994 PA, only the ramps to the disposal area were assumed to be backfilled and effectively sealed.

Backfill was not used in either the access drifts or directly around the waste parcel for either the horizontal or vertical emplacement schemes. An air gap was selected in place of backfill-buffer material. The radiative heat transfer through the air gap is more effective than the heat transfer through the crushed-tuff backfill-buffer. The trapped air in crushed-tuff backfill-buffer, which has a low thermal conductivity, would act as an insulator thus increasing centerline temperatures.

How the air gap around the waste parcel was modeled depends on modeling capabilities and intended effects, and was treated in several different ways. For the calculation of heat transport directly around the waste parcel, an

** The term "backfill-buffer" is used to denote backfill placed around a waste parcel. The term was used in the report of the 1993 PA because backfill around a waste parcel in granite was expected to moderate the release of contaminants to the host rock. Note that a 2.54-cm air gap is modeled around the waste parcel in the 1994 PA.

Table 6-4. Differences between Horizontal and Vertical Orientations for Waste Emplacement in Repository

	Horizontal	Vertical
Repository Layout	<ul style="list-style-type: none"> - Regular rectangular system of parallel waste disposal rooms - Drift length constant (426.0 m) 	<ul style="list-style-type: none"> - Same
Waste Parcels (discussed in Chapter 4)	<ul style="list-style-type: none"> - Multi-Purpose Canister (MPC) for spent fuel - MPC for high-level waste includes four DOE standard canisters 	<ul style="list-style-type: none"> - Legal Weight Truck (LWT) for spent fuel - DOE standard canister for high-level waste
Waste Disposal Room	<ul style="list-style-type: none"> - Circular cross-section; 4.3 m diameter - Rail system for transporting MPC inside drifts - No backfill - 59 rooms 	<ul style="list-style-type: none"> - Semi-circular/semi-rectangular cross section; 3.81-m radius of dome ceiling; 7.62-m high, 7.62-m wide rectangular base - No backfill - 38 rooms
Waste Parcel Boreholes	N/A	<ul style="list-style-type: none"> - 2.54-cm annulus air gap - Borehole for LWT; 0.751 m diameter; 5.5 m depth - Borehole for DOE standard canister; 0.635 m diameter; 4.0 m depth - Hexagonal 2.6-m center to center, 3-row borehole spacing - Radiation (gamma) shielding plug, 1.0-m thick (from waste disposal room floor to top of waste parcel in borehole)
Access Drifts	<ul style="list-style-type: none"> - Semi-circular/semi-rectangular cross section (dome-shaped ceiling with rectangular base) - Width: 7.62 m - Height: 7.62 m - Backfilled with crushed tuff after emplacement 	Same, but no backfill
Repository Design Considerations	<ul style="list-style-type: none"> - Highest possible areal power density (23.5 W/m²) - Tunnel Boring Machine (TBM) for mining rooms - Thermal constraints <ul style="list-style-type: none"> - host rock/waste parcel interface temperature below 200°C - maximum centerline temperature below 350°C in waste parcel (200°C for ATR fuel) 	<ul style="list-style-type: none"> - 14.1 W/m² areal power density - Tunnel Boring Machine (TBM) for mining rooms and access drifts - Thermal and geometric constraints <ul style="list-style-type: none"> - host rock/waste parcel interface temperature below 100°C - rock stability for drilling boreholes

analytic solution for radiative heat transfer through the air gap was used; potential vaporization of water was neglected. For the calculation of one-phase fluid flow, the porosity of the air gap was added to the fracture porosity and a continuum assumed between the waste parcel and the host rock. For the calculation of coupled two-phase flow and thermal calculations in the Complex PA, the porosity of the gap was added to the fracture porosity in the grid. Thus, the thermal calculations in the Complex PA did not consider radiative heat transfer through the gap but allowed for potential vaporization of the water. For the source term calculations, both intact air gaps and gaps filled with rubble from degradation of the tunnel over time were considered because (1) the presence of the rubble meant that, in addition to dripping, the matrix could have contact with water percolation, and (2) a diffusion pathway through the rubble was a potentially important release mechanism for radionuclides.

Table 6-5. Waste Unit Factors for Hypothetical Repository for Simple PA

Waste Type	WP ID No.	Total Activity (Ci)	No. of WP used in Complex PA	Original Waste Factor	No. of WP used in Simple PA	Equivalent Waste Factor	Area of Disposal Region used in Simple PA (m ²)
Horizontal							
Graphite SNF	101	4.291×10^6	83	2.8×10^{-2}	2818	0.9507	6.4113×10^4
N-Reactor SNF	102	3.3040×10^7	59	2.1	2818	100.3017	6.4113×10^4
Shippingport SNF	103	1.744×10^8	256	1.1×10^{-1}	3140	1.3492	7.1440×10^4
ATR (HEU) SNF	104	4.0910×10^7	33	7.2×10^{-2}	2657	5.7971	6.0449×10^4
PWR (LEU) SNF	105	2.0670×10^7	36	1.62×10^{-1}	2514	11.3130	6.0449×10^4
INEL Calcine Glass-Ceramic HLW	106	1.4960×10^7	2037	3.2×10^{-1}	4605	0.7234	7.3272×10^4
DOE Savannah HLW	107	1.1740×10^9	1321	8.036	4605	28.0135	7.3272×10^4
DOE Hanford HLW	108	5.0450×10^8	490	1.16	4605	10.9016	7.3272×10^4
DOE West Valley HLW	109	3.0120×10^7	69	7.15×10^{-2}	4605	4.7718	7.3272×10^4
INEL Calcine Borosilicate Glass HLW	110	1.4960×10^7	7249	3.2×10^{-1}	4605	0.2033	7.3272×10^4
INEL Calcine Loose HLW	111	1.4960×10^7	1737	3.2×10^{-1}	4605	0.8484	7.3272×10^4
Vertical							
Graphite SNF	201	4.291×10^6	560	2.8×10^{-2}	18645	0.9323	1.2660×10^5
N-Reactor SNF	202	3.3040×10^7	394	2.1	18645	99.3769	1.2660×10^5
Shippingport SNF	203	1.744×10^8	1540	1.1×10^{-1}	18645	1.3318	1.2660×10^5
ATR (HEU) SNF	204	4.0910×10^7	233	7.2×10^{-2}	18645	5.7615	1.2660×10^5
PWR (LEU) SNF	205	2.0670×10^7	252	1.62×10^{-1}	18645	11.9861	1.2660×10^5
INEL Calcine Glass-Ceramic HLW	206	1.4960×10^7	8147	3.2×10^{-1}	18645	0.7323	1.2660×10^5
DOE Savannah HLW	207	1.1740×10^9	5283	8.036	18645	28.3610	1.2660×10^5
DOE Hanford HLW	208	5.0450×10^8	1960	1.16	18645	11.0348	1.2660×10^5
DOE West Valley HLW	209	3.0120×10^7	276	7.15×10^{-2}	18645	4.8301	1.2660×10^5
INEL Calcine Borosilicate Glass HLW	210	1.4960×10^7	28994	3.2×10^{-1}	18645	0.2058	1.2660×10^5
INEL Calcine Loose HLW	211	1.4960×10^7	6945	3.2×10^{-1}	18645	0.8591	1.2660×10^5

6.4 Summary of Modeling Assumptions for Repository Design

- Repository is rectangular with parallel waste disposal rooms and access drift that runs along perimeter.
- Access drift for people and machinery runs along length of repository and leads to ramps to surface facilities.
- Waste disposal rooms are 426-m long.
- Two waste emplacement orientations are considered: horizontal (indrift) and vertical (borehole).
- 14.0 W/m^2 was used as design-basis areal power density for vertical emplacement.
- 23.5 W/m^2 was used as a design-basis areal power density for horizontal emplacement.
- Horizontal emplacement: 59 waste disposal rooms, 125-ton MPCs on rail system, no backfill in room.
- Vertical emplacement: 38 waste disposal rooms, 25-ton LWT containers (spent fuel) and DOE standard containers (high-level waste), 2.6-m center to center spacing, 2.54-cm air gap between waste parcel and host rock, containers sit on bottom of borehole, shield plug and cover plate over container, no backfill in room.

7. Scenario* Development

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Evaluating the performance of a disposal system requires not only a scientific understanding of the current system but also a prediction of its behavior for 10,000 yr. Consequently, models must be developed to simulate plausible futures of the disposal system. Scenario development is the second phase of conceptual model development (the first being disposal system characterization, Chapters 4 through 6). In conjunction with system characterization, the scenario development process establishes how the real world will be represented by conceptual model(s).

Generally speaking, scenario development is the process of deciding what may happen to the disposal system in the future and how to model it. The process entails selecting features (e.g., an area where precipitation collects at the surface and infiltrates into the tuff), events (e.g., humans drilling into the repository), and processes (e.g., corrosion of containers in the repository after disposal of the waste). At this level, scenario development consists of several steps:[†]

1. Identifying the full scope (i.e., "universe") of features, events, and processes of the disposal system. (Events are also referred to as short-term phenomena; processes, as long-term phenomena.)
2. Selecting for the model those features, events, and processes that might contribute to contaminants being released to the accessible environment. (Regulations and standard modeling practice guide the selection process. For example, regulatory guidance indicates that some events may be discarded, and standard modeling practice is to assume that most aspects of the biosphere persist for 10,000 yr.)
3. Creating conceptual models based on (a) the disposal system characterization and (b) the selected features, events, and processes.
4. Incorporating those conceptual models into the performance assessment calculations.

During the scenario development phase, many decisions are made about what to include in the model. However, the decisions themselves are more conveniently discussed in the chapters that describe either system characterization or consequence models. For example, features included are discussed in the chapters on geologic and engineered barriers (Chapters 4, 5, and 6); processes and events are discussed with the consequence models (Chapters 9 through 14).

This chapter summarizes the process of identifying and selecting the features, events, and processes, including an overview of the results, and describes the design selected for the 1994 performance assessment calculations.

7.1 Identification and Selection of Features, Events, and Processes

7.1.1 Summary of Features, Events, and Processes Selected for Study

The basic features, events, and processes selected for modeling in the 1994 PA are briefly summarized below.

* In this chapter, the noun "scenario" is a synonym for the term "the set of all features, events, and processes considered for incorporation in the conceptual model of the disposal system." Other meanings of "scenario" are described in Sections 3.3.1 and 3.3.2; instances of the use of one of these other meanings in this chapter are noted by citation to Sections 3.3.1 or 3.3.2.

† Other authors have used the term scenario development to refer to steps 1 and 2 only, because these two steps initially exact greater attention than steps 3 and 4. In this report, however, scenario development includes not only the selection of the features, events, and processes but also the incorporation of those components into the computational model.

7. Scenario Development

Features. As described in Chapters 5 and 6, the basic features explored are (1) an area where precipitation collects at the surface and infiltrates into the tuff; (2) a highly fractured, pancake stratigraphy; (3) a large unsaturated zone in which the repository is located; (4) vertical and horizontal emplacement of waste containers; and (5) an underlying aquifer. All features are assumed to be present with certainty, i.e., no undetected features are considered. The location of a collection point for precipitation is assumed to be known with certainty; only the magnitude of the precipitation is assumed uncertain and is treated as a process along with climate variability. Details of features included near the containers and within the containers are described in Chapters 4 and 11. Simplifying assumptions are also discussed in the corresponding chapters.

Events. The basic events considered in this performance assessment were the same as those identified for Yucca Mountain by Barnard et al. (1992) and Wilson et al. (1994). However, only three of these events are used to form summary scenarios (Section 7.1.2) in the present study: they are (1) human intrusion through exploratory drilling, (2) basaltic volcanism, and (3) repository criticality. Some aspects of the last of these have been treated as a process in the present study.

Processes. Basic processes explored for the geologic barrier, waste form, waste container, and repository are as follows:

- *Geologic Barrier.* Processes considered are two-phase flow and heat conduction with possible phase change in a fractured matrix, large sorption of selected radionuclides on tuff, and infiltration variations from climate change, with amount focused on center of the repository.
- *Waste Form.* The process considered is control of radionuclide release by solubility; matrix alteration or immediate release of some radionuclides in gaps and grain boundaries of spent fuel and degradation of cladding and matrix containing radionuclides (except for fuel and initially failed cladding).
- *Waste Container.* Processes considered are gas consumption from several layers because of generalized oxidic corrosion, radionuclide release through containers as controlled by localized corrosion, and diffusion through container breach into the host rock.
- *Repository.* The process considered is radiative heat transfer through an air gap between the container and the host rock.

Table 7-1 lists these processes and also identifies differences in processes between the Simple and Complex PA modeling of the geologic barrier. These differences are discussed in Section 7.2. The simplifying assumptions for the processes are included in the discussion of the consequence models, Chapters 9 through 14.

The idea of a summary scenario is explained in Section 3.3.1 and in more detail in Tierney (1991, p. 3-22 to 3-26). Summary scenarios are most easily identified through use of a logic diagram (for instance, Figure 3-12) in which the various possible sequences of events and undetected features are enumerated and their probabilities computed.

In the present study, three events were judged to be important in enumerating summary scenarios: human intrusion by exploratory drilling (HI); basaltic volcanism (V); and repository criticality (C). All other events, processes, and features were treated as either certainties or impossibilities. The summary scenarios arising from these three events are enumerated in Figure 7-1; the remainder of the discussion of these summary scenarios will rely heavily on this figure.

It is seen that there are eight summary scenarios, $S_0, S_1, \dots, S_7$, with S_0 denoting the base case in which none of the potentially disruptive events (HI, V, C) occurs. The physical meaning of each S_n can be seen by tracing a path through the logic diagram from the starting point $t = 0$ in Figure 7-1 to one of the terminal points at $t = 10,000$ yr; for example, S_7 denotes the scenarios in which HI, V, C each occur at least once in the 10,000-yr period.

Enumeration of summary scenarios by logic diagram also affords a straightforward way of calculating the probabilities of the summary scenarios, in this case denoted by $P(S_n)$, $n = 0, 1, \dots, 7$, in terms of the elementary probabilities of occurrence of the base events. In the present work, the elementary probabilities of the base events are defined as follows:

Table 7-1. Simplifications of Phenomena Modeled in Unsaturated Flow and Transport Codes

System Component	Phenomenon	Simplification	
		Complex PA	Simple PA
Geologic Barrier	Climate variability	Sinusoidal increase	Steady state at average of sinusoidal increase
	2-phase flow and heat transport with phase changes	2-D, 2-phase flow and heat conduction with water phase change	2-D gas flow decoupled from 3-D heat conduction and radiative heat transfer, which are both decoupled from 1-D liquid flow and transport; no phase changes
	Large sorption of selected radionuclides	Linear isotherm (Kd) not a function of temperature (temperature pulse usually diminished by time containers fail)	Same
	Exchange of $^{14}\text{CO}_2$ with bicarbonate in solution (H_2CO_3^*)	Approximated with effective Kd	Same
	Fracture and matrix flow	2-D, 2-phase, composite porosity in unsaturated zone; 3-D, single-phase, dual porosity in saturated zone	1-D, single-phase, composite porosity in unsaturated zone; fracture and matrix fluid velocities approximated from composite velocity to use dual-permeability transport Distribution of travel times from 3-D, single-phase, dual porosity in saturated zone.
Engineered Barrier Repository	Oxygen may not be drawn fast enough from surface to keep repository oxic, because O_2 could become depleted by reaction with carbon steel inside container, producing a reducing environment and low radionuclide solubilities, corrosion rates.	O_2 always assumed to be present	Same
	Air gap between container and host rock (at emplacement)	Volume of air gap included in porosity of fractures in disposal region	Included only in source model.
	Collapse of rooms and boreholes allows rubble to come in contact with containers, hastening corrosion through direct contact with partially saturated tuff matrix	Variable fraction of containers assumed to be in contact with matrix	Same

Table 7-1. Simplifications of Phenomena Modeled in Unsaturated Flow and Transport Codes (Continued)

System Component	Phenomenon	Simplification	
		Complex PA	Simple PA
Waste Parcel Waste Form	Release of ^{14}C from gaps in fuel	Compartment with quick release fraction of ^{14}C	Same
	Spent fuel with failed cladding	Fraction of spent fuel missing cladding	Same
	Release controlled by solubility and degradation of matrix containing radionuclides	Alteration rate used to control degradation, released radionuclides, placed in compartment for release through solution	Same
Waste Container	Diffusion through partially failed layers impedes release of radionuclides	Release controlled by effective diffusion area through container	Same
	Several protective metallic layers generate gas when corroded	Alteration rate used for corrosion; corrosion can partially fail layer and allow corrosion of newly exposed layer while corrosion on first layer continues	Same
	Portion of containers may contain defects	Fraction of containers have outer, failed layer	Same
	Containers often fail through localized corrosion	Only fraction of mass of protective layer must corrode before layer designated as "failed"; fraction depends on material.	Same
	Radionuclides can adsorb onto iron particles from corroded container	Sorption through linear isotherm (K_d)	Same

P_1 = probability that HI occurs at least once in 10,000 yr;

P_2 = probability that V occurs at least once in 10,000 yr,

P_3 = probability that C occurs at least once in 10,000 yr.

These elementary probabilities are assigned in Chapter 8, or taken from other sources. The quantity P_1 , the elementary probability of human intrusion, is taken as $\sim 7.93 \times 10^{-2}$. The elementary probabilities of basaltic volcanism, P_2 , is conservatively taken as 2.4×10^{-4} on the basis of Barnard et al. (1992, p. 7-5 to 7-7). The elementary probability of repository criticality, P_3 , is taken as 1.6×10^{-2} (see Section 8.5).

The resulting probabilities of the summary scenarios, the $P(S_n)$, are given on the right-hand side of Figure 7-1. It is seen that scenarios S_3 , S_6 , S_7 , and (marginally) S_2 can be ignored in calculating a total complementary cumulative

Figure 7-1. Logic diagram to enumerate summary scenarios considered in the 1994 PA. HI = human intrusion by exploratory drilling; V = basaltic volcanism; C = repository criticality. p_1 , p_2 , p_3 are probabilities of at least one occurrence of HI, V, C, respectively, in a 10,000-yr term. S_i , $0 \leq i \leq 7$ labels the summary scenarios; $P(S_i)$ are probabilities of the summary scenarios. See text for sources of numerical values of the $P(S_i)$.

distribution function (CCDF) for the 1994 PA by virtue of the EPA guidance that allows omission of categories of events, processes, and features that have probabilities of occurrence in 10,000 yr of less than 10^{-4} . Eliminating S_2 , S_3 , S_6 , and S_7 leaves the base case scenario (S_0), a scenario involving only repository criticality (S_1), a scenario involving only human intrusion (S_4), and a scenario involving repository criticality and human intrusion (S_5). In Chapter 10, the criticality event is divided further into moderated/unmoderated and fast/slow categories.

7.2 Calculational Design

The scenario development phase of model conceptualization must conclude with models of selected features, events, and processes that are computationally feasible in order to predict future consequences. This section provides details about the calculation design. One aspect of the design, the number of parameters to be varied, is discussed in Chapter 8, "Probability Modeling."

7.2.1 Submodels of the Consequence Model

For the 1994 PA, the consequence model was divided into six major groups of computational models (submodels), which are discussed in the indicated chapters:

1. Cuttings code for direct release to surface (Chapter 9).
2. Criticality safety codes for evaluating critical conditions (Chapter 10).
3. Codes for evaluating corrosion and release of radionuclides from containers (Chapter 11).
4. Flow and transport codes for predicting radionuclide movement in unsaturated portion of lithosphere (Chapters 12 and 13).
5. Flow and transport codes for predicting radionuclide movement in saturated portion of lithosphere (Chapters 12 and 13).
6. Biosphere transport code (Chapter 14).

These modeling categories were created to address particular aspects of the calculation design. The cuttings category was separate from the fluid flow category based on the assumption that the drilling did not affect fluid flow around the repository because the tuff is already highly fractured. (The same assumption was made for the granite disposal system in the 1993 PA and for performance assessments for the Yucca Mountain Project, but it has not been evaluated thoroughly.) The criticality modeling was also separated from the main modeling system because of a decision during scenario development to consider critical conditions as a separate scenario (see Section 7.2.2 and Chapter 10). The corrosion group of computational models was formed in response to the large amount of data required to simulate container corrosion and subsequent escape of radionuclides. The flow and transport categories were grouped by unsaturated and saturated conditions, which are convenient subdivisions of the geologic barrier. Finally, the biosphere codes were grouped to determine human dose, which represents a set of release criteria different from that determined by the flow and transport codes.

Modeling efforts for cuttings, criticality, and transport were generally performed in parallel. Figure 7-2 provides a general overview of the calculational design and shows the paths of information for the 1994 PA, including steps performed in parallel.

7.2.2 Levels of Process Simplification for Transport in Lithosphere

Whenever a system is analyzed through modeling, physical phenomena, such as physical processes in the repository and the host rock, are simplified. Although the level of simplification that is appropriate cannot always be known *a priori*, evaluating the correct level of simplification is an important task.

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Figure 7-2. Sequence of calculations showing Simple and Complex PA consequence calculations done in parallel (see also Figure 1-1).

In the 1994 PA, two levels of simplification were used to model the transport of radionuclides in the lithosphere. The purpose of using two levels is to compare results and to explore the level of simplification that is appropriate for rapid response to future questions regarding alternative waste-treatment options. The first level is referred to as the "Simple PA" and the second as the "Complex PA." The terms simple and complex are relative only to each other; compared to many risk assessments, the Simple PA is quite detailed.

Simple PA. In the 1993 PA, the primary goal of a Simple PA was to use a level of simplification that allowed simulations to be set up quickly and geared toward fast run times, relative to the Complex PA. In the 1994 PA, the primary goal was to adopt models and methods similar to those used in TSPA-1993 (Wilson et al., 1994), which in turn had fast run times as a goal. Therefore, in the Simple PA, one waste type (e.g., graphite spent fuel) could be studied in the repository at a time, in addition to a mix of all waste types. Eleven single waste parcels were studied, including three INEL high-level waste forms: calcined waste in a glass-ceramic matrix, in borosilicate glass, and in loose granular form. The computational models (i.e., codes) used in the Simple PA are shown in Figure 7-3 superimposed over the basic features that they model.

7. Scenario Development

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Figure 7-3. General conceptual model for tuff disposal system for the Simple PA. The schematic includes the main features and the corresponding computational models (codes). Although features are shown in two dimensions, they were actually modeled in one dimension for the Simple PA.

In the 1993 PA, the mathematical description of the conceptual model was made using a sophisticated set of ordinary differential equations to arrive at a lumped parameter model. In the 1994 PA, the method of modeling the phenomena was distinctly different. Specifically, the description of the natural phenomena consisted of (a) numerical solutions of one-dimensional versions of the mathematical model (e.g., the one-dimensional single-phase code, TOSPAC, was used [Dudley et al., 1989]), or (b) abstractions of results from detailed phenomenological models similar to those used in the Complex PA.[‡] The second method was used for evaluating transport of $^{14}\text{CO}_2$ in the unsaturated zone, where analytic curve fits to a two-dimensional analysis of gas movement driven by temperature increases were used, and for characterizing the transport results in the saturated zone obtained from the Complex PA. In the latter application of model abstraction, the path lengths and travel times of a neutrally buoyant particle were characterized as a distribution of path lengths and velocities, which were then placed in a one-dimensional single-phase analytic code for evaluating transport of nonsorbing, but decaying, radionuclides.

The consequence models used in the Simple PA are discussed in Chapter 13 and listed in Appendix G.

Complex PA. The Complex PA used detailed phenomenological simulation codes. The codes for the Complex PA and the basic features they model are shown in Figure 7-4. The codes were based on mathematical models with potentially spatially distributed model parameters and used partial differential equations (PDEs) that were solved numerically on coarse grids. The regulatory performance criteria were evaluated directly from multiple execution of the simulation codes and thus provided a direct connection between the input data and the performance criteria. (When model abstraction is used to arrive at the simplification, as in this year's Simple PA, this connection can become somewhat obscure.)

The waste types, including all the spent fuels and the INEL high-level waste as a glass-ceramic, were studied as a group and with minimal treatment. In addition, high-level waste in borosilicate glass from three DOE sites (Savannah River, Hanford, and West Valley) was included. In the Complex PA, the waste was uniformly distributed in the repository.

The consequence models used in the Complex PA are discussed in Chapter 12 and listed in Appendix G.

7.2.3 Modeling System Assembled

In a performance assessment, many categories of software are needed to complete the task. These categories basically reflect the fundamental steps of a performance assessment (see Chapter 1, Figure 1-1, and Figure 7-2). The categories that must be considered in a performance assessment are modeling setup, consequence modeling, probability modeling, compliance assessment (CCDF construction), and sensitivity analysis. For the 1994 PA, probability modeling and compliance assessment are grouped together. Also, consequence modeling is divided into six submodels as described in Section 7.2.1.

The submodels for the Complex and Simple PAs and how they are linked are shown in Figures 7-5 and 7-6, respectively. The linkage of this software is by means of CAMCON (Rechard, Ed., 1992; Rechard et al., 1993). (Support codes that are used with the main modeling codes are not depicted in these figures but can be found in the detailed figures in Appendix G. Version numbers and a functional description of each code are also provided in Appendix G.) The categories of software required by the 1994 PA are described below.

Modeling Setup. The main function of the modeling setup is modeling parameter input. The processes for parameter selection are the following: (1) select parameter values and distributions ($\mathbf{x} = \mathbf{x}_1, \dots, \mathbf{x}_N$) consistent with the manner of use in models; (2) place parameter values in secondary data base (INGRES®) for use by models; (3) select subset of parameters to vary (parameter uncertainty) (see Chapter 8), and (4) sample with Latin Hypercube sampling (LHS) (Iman and Shortencarier, 1984).

[‡] It was not the purpose of this report to examine the utility of using model abstraction to arrive at simple models. Rather, as previously stated, the goal was to approximate the techniques of TSPA-1993 (Wilson et al., 1994).

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Figure 7-4. General conceptual model for tuff disposal system for the Complex PA. The schematic includes the main features and the corresponding computational models (codes).

*GENII-S both Simulates Biosphere Transport and Summarizes Results

TRI-6342-3577-1

Figure 7-5. Modeling system for Complex PA.

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Figure 7-6. Modeling system for Simple PA.

Cuttings Consequence Modeling. The code used to predict the amount of cuttings/cavings reaching the surface from an exploratory drilling is WPRD, a modified version of the CUTTINGS code that was used in the 1993 PA.

Radionuclide Source-Term Consequence Modeling. This software group evaluates the amount of gas consumed during corrosion and release of radionuclides to the host rock as the containers fail. The two codes in this category are GASSNF and USATCONC. They are called directly by the unsaturated zone consequence modeling codes discussed below.

Unsaturated Zone Consequence Modeling. This software group evaluates radionuclide movement in the unsaturated zone of the tuff disposal system. For the Complex PA, BRAGFLO_T and NUTS are the primary modeling codes, solving the heat conduction and two-phase flow equations on a coarse two-dimensional finite-difference grid. For the 1994 PA, the composite-porosity formulation (which is described in Chapter 12) was added to BRAGFLO_T. NUTS is a new code for unsaturated transport that uses BRAGFLO_T velocity fields.

For the Simple PA, SUMQ_3D and CONRAD were used to analytically evaluate the temperature field within and around the repository. In the 1994 PA, the results of these codes are used by USATCONC to determine corrosion rates, which depend upon temperature. TOSPAC (Dudley et al, 1989), the one-dimensional finite-difference modeling code from Yucca Mountain Project's TSPA-1993 (Wilson et al., 1994) was then used for liquid transport after it was coupled with the WIPP modeling system, CAMCON (Rechard, Ed., 1992; Rechard et al., 1993). For gas transport, an abstraction of the two-dimensional results from TSPA-1991 (Barnard et al., 1992) was accomplished using GASTP, a curve-fitting code that was developed specifically for the 1994 PA.

Saturated Zone Consequence Modeling. This group of software models the transport of radionuclides in the saturated zone of the tuff disposal system. The source term considered is radionuclides that reach the water table. Because the geologic barrier in the 1994 PA is tuff, the applied model is completely changed from the model used in the 1993 PA. For the Complex PA, an important change was the construction of a three-dimensional model of the aquifer, similar to that used in TSPA-1993. Thus the code STAFF3D was used in the 1994 PA rather than STAFF2D, which was used by the 1993 PA. For the Simple PA, equivalent velocity and distribution from TSPA-1993 (Wilson et al., 1994) were used as input to QEDTP for transporting radionuclides in one dimension.

Biosphere Consequence Modeling. This software group evaluates transport of radionuclides in the biosphere in the accessible environment using GENII-S (Leigh et al., 1993; Napier et al., 1988a,b,c). GENII-S also determines the radionuclide dose to humans (a performance measure) and so is also displayed as a results analysis code (Figure 7-6). This software was included only as a demonstration in the 1993 PA.

Probability Modeling and CCDF Construction. This group of software evaluates the probability of human intrusion for exploratory drilling and constructs the CCDF for both normalized releases and doses. Only minor differences exist between the 1993 and 1994 versions. The changes (for example, allowing for variable drill bit diameters) were intended to improve the flexibility of the codes.

Sensitivity Analysis. As the name implies, this group of software evaluates parameter importance through sensitivity analysis by determining the partial correlation coefficients and standardized regression coefficients. The main codes are STEPWISE (Iman et al., 1980) and PCCSRC (Iman and Helton, 1985). No changes occurred from the 1993 PA.

Criticality Modeling. This software group was not directly coupled to CAMCON and so is not shown in Figure 7-6. Two criticality codes were used: MCNP (Briesmeister, 1986, 1988) and KENO_V (ORNL, 1984). In addition, RNK is a modeling code developed for the 1994 PA to explore the nuclear dynamics of the criticality scenario, which is very important in evaluating whether the operation of an assembly of fissile material can be maintained.

7.2.4 Cases Simulated without Critical Conditions

The simulations for the 1994 PA fall into two main groups: (1) cases that evaluate aspects of a criticality in or around waste parcels and (2) cases that evaluate radionuclide releases to the accessible environment from plausible conditions in the future, including climatic change and human intrusion through exploratory drilling. As described in Section 7.2.1 and Chapter 10, the first group is considered as a single group of submodels that is used to model critical conditions. The second group is similar to the 1993 PA, except that only minimal treatment options were examined instead of multiple treatment options. A summary of these cases is provided here.

As described in Section 7.2.1, the consequence model for the second group of simulations contains several submodels. Also, as described in Section 7.2.2, transport in the unsaturated and saturated zones of the tuff disposal system were run with two levels of simplification. Different cases were run for the Complex and Simple PAs (Table 7-2).

Table 7-2. Cases Run to Evaluate DOE Waste in Tuff Disposal System, Assuming No Critical Conditions

Waste Parcel ID		Description	Cuttings	Submodels Unsaturated and Saturated Transport		Biosphere Transport
Horizontal	Vertical			Simple PA	Complex PA	
101	201	Spent nuclear fuel (SNF), graphite, Fort St. Vrain	x	x		
102	202	SNF, weapon production fuel, N-Reactor	x	x		
103	203	SNF, robust highly enriched uranium (HEU), Shippingport	x	x		
104	204	SNF, HEU, Advanced Test Reactor (ATR)	x	x		
105	205	SNF, low enriched uranium (LEU), pressurized water reactor	x	x		
106	206	High-level waste, (HLW) INEL calcine in glass ceramic	x	x		
107	207	HLW, borosilicate glass, Savannah River	x	x		
108	208	HLW, borosilicate glass, Hanford	x	x		
109	209	HLW, borosilicate glass, West Valley	x	x		
110	210	HLW, INEL calcine, loose	x	x		
111	211	HLW, INEL calcine, in borosilicate	x	x		
100 Waste disposal group (Waste Parcels 101-109)			x	x	x	x
200 Waste disposal group (Waste Parcels 201-209)			x	x	x	x

• See also Chapter 4, Waste Parcel Description

1 For the Complex PA in 1994, the groundwater-release consequence submodel was used to simulate a uniform
2 distribution of all the waste types in the waste disposal rooms of the repository. The advantages of modeling the
3 waste types together are that (1) fewer calculations were required, and (2) synergistic effects between waste forms are
4 possible. In regard to the latter advantage specifically, (a) heat generation and oxygen consumption are more repre-
5 sentative of an actual repository and (b) robust waste forms can moderate the impact of nonrobust waste forms on the
6 total radionuclide release.
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9 The Simple PA in 1994 simulated the effects of placing single waste types in a repository. Twenty-two cases (11
10 each for horizontal and vertical orientation of the waste parcels) were simulated. The advantages of modeling a sin-
11 gle waste parcel per repository are that (1) results are easily compared and, thus, the performance of the waste types is
12 easily ranked, and (2) the acceptability of placing individual waste types in a repository is easy to evaluate.
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8. Probability Modeling

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A probability model estimates the likelihoods of uncertain parameter values and also the likelihood of the events and processes of a scenario (Section 3.2.3). Although a probability model can be a computer algorithm, in this report it is either (1) an analytic function or (2) a subjective distribution estimated by experts and analysts. For instance, the Poisson analytic function provides the estimation of the probability of the event of inadvertent human intrusion into the tuff repository—essentially the same as reported for the 1993 PA.

This chapter lists and depicts the distributions of the parameters selected to be varied from among the approximately 3000 model parameters, and describes the analytic function chosen by the experts or analysts to present these uncertain parameters. However, the basis for these estimates is found in the chapters in which the specific parameters are discussed (e.g., Chapter 11, Gas Consumption and Source Term Submodels) rather than here. Also, the fault tree for evaluating the probability of critical conditions in the repository is described in Chapter 10, instead of in this chapter, so that the discussion of criticality dynamics is self-contained.

8.1 Model Parameters

Model parameters ($x = x_1, \dots, x_n, \dots, x_{nV}$) are the underlying fundamental entities of computational probability and consequence models (see Sections 3.2.1 and 3.2.2). For this performance assessment, they are all scalar quantities and are all coefficients in the mathematical models underlying the computational models.

8.1.1 Characterizing Parameter Uncertainty

Characterizing the uncertainty in x requires developing a joint probability distribution, $F(x)$; usually, the joint distribution is approximated by the product of distributions of the individual parameters ($F(x_1) \cdot F(x_2) \cdot \dots \cdot F(x_{nV})$) (i.e., the parameters are assumed to be independent of each other). These individual distributions may be defined by probability density or cumulative distribution functions (PDFs or CDFs; see below). The distribution (either CDF or PDF) of a parameter, x_n , ideally represents both what we know and what we do not know about that parameter and should reflect the best, current knowledge of the range and likelihoods of the appropriate parameter value when used in a consequence or probability model. It is possible that the $F(x_n)$ may be obtained by classical statistical techniques for some parameters. However, in many cases, each $F(x_n)$ will be a subjective distribution based on the degree of belief that is developed from available information through a suitable review process.

For a continuous parameter, say X , the *probability density function* (PDF) is a function $f(x) > 0$ with the properties

$$\int_a^b f(x) dx = \text{probability that uncertain parameter } X \text{ lies in interval } (a,b):$$

$$\int_{-\infty}^{+\infty} f(x) dx = 1.$$

The *cumulative distribution function* (CDF) associated with $f(x)$ is defined by

$$F(x) = \int_{-\infty}^x f(s) ds = \text{probability that uncertain parameter } X \text{ is less than or equal to } x.$$

8. Probability Modeling

Probability density functions (PDFs) and CDFs can be similarly defined for uncertain parameters that take on a denumerable number of values, x_i , $i=1,2, \dots$. The sequence $\{f_i\}$, $i=1,2, \dots$, such that $f_i > 0$ and

$$\sum_i f_i = 1,$$

is the discrete analogue of the continuous PDF, and

$$F(x) = \sum_{\text{all } x_i < x} f_i$$

is the discrete analogue of the continuous CDF.

Range. The range of a distribution is denoted by (a,b) , the pair of numbers in which a and b are respectively the minimum and maximum values that can reasonably be taken by the uncertain parameter X .

Mean and Sample Mean. The mean value (or, simply, *mean*) of a distribution is one measure of the central tendency of a distribution; it is analogous to the arithmetic average of a series of numbers. The population mean, μ , is defined by

$$\begin{aligned} \mu &= \int_{-\infty}^{\infty} x f(x) dx \quad \text{for continuous distributions} \\ &\text{or} \\ &= \sum_{\text{all } x_i} x_i f_i \quad \text{for discrete distributions.} \end{aligned}$$

The *sample mean*, denoted by $\bar{x}$, is the arithmetic average of values in an empirical data set.

Median and Sample Median. The *median* value of a CDF is denoted by x_{50} and is that value in the range at which 50% of all values lie above and below (i.e., the 0.5 quantile). *Sample medians*, here denoted by $\bar{x}_{50}$, can be obtained directly from empirical CDFs.

Variance and Coefficient of Variation. The *variance* of a distribution, σ^2 , is the second moment of the distribution about its mean, i.e.,

$$\begin{aligned} \sigma^2 &= \int_{-\infty}^{\infty} (x - \mu)^2 f(x) dx \quad \text{for continuous distributions} \\ &\text{or} \\ &= \sum_{\text{all } x_i} (x_i - \mu)^2 f_i \quad \text{for discrete distributions.} \end{aligned}$$

The *standard deviation*, σ , is the positive square root of the variance. The coefficient of variation, the ratio of standard deviation to mean, σ/μ , is a convenient measure of the relative width of a distribution.

The *sample variances* of a set of measurements of parameter x_n , say $x_1, x_2, x_3, \dots, x_n$ is the sum

$$s = \frac{1}{(nV-1)} \sum_{n=1}^{nV} (x_n - \bar{x})^2.$$

The sample variances of independent measurements of some quantity is an unbiased estimator of the population variance of that quantity (Blom, 1989, p. 197). Although the mean, median, and variance can be formally calculated for empirical CDFs derived from subjective estimates of experts, these are not truly sampled means, medians, and variances and therefore these are not calculated in this study.

Categories of Distributions. Distributions used in this report are grouped into four categories:

1. Continuous analytical distributions: normal, lognormal, uniform, loguniform, or beta (Table 8-1),
2. Discrete analytical distributions: Poisson (Table 8-1),
3. Constructed distributions based on judgment ("Subjective Estimates"),
4. Miscellaneous categories (null distributions): constant, and tabular.

Continuous Distributions. Five continuous, analytical distributions used in this report are described below.

Normal. Normal designates the normal PDF, a good approximation to the distribution of many physical parameters. The normal distribution arises naturally from the central limit theorem (Johnson and Kotz, 1970, p. 40; Miller and Freund, 1977, p. 104). For purposes of performance assessment, the distribution is arbitrarily truncated at the 0.01 and 0.99 quantities (i.e., the probability that the parameter will be smaller or larger is 1%), which corresponds to $\bar{x} \pm 2.33s$, where s is the sample standard deviation.

Lognormal. Lognormal designates a lognormal PDF, a distribution of a variable whose logarithm follows a normal distribution. Like a normal distribution, the lognormal distribution is arbitrarily truncated at the 0.01 and 0.99 quantiles.

Uniform. Uniform designates a PDF that is constant in the interval (a,b) and zero outside of that interval.

Loguniform. Loguniform designates a loguniform PDF, a distribution of a variable whose logarithm follows a uniform distribution.

Beta. Beta designates a versatile PDF, specified by two parameters that can assume numerous shapes in a specified range (a,b) (Harr, 1987, p. 79; Johnson and Kotz, 1970, p. 37; Miller and Freund, 1977, p. 119). The beta distribution was not used in the 1993 PA. In the 1994 PA, however, many model parameters for the geologic barrier that originated in TSPA-1993 (Wilson et al., 1994) were originally described by beta distribution and thus were used here also, since re-evaluation of these model parameters was beyond the scope of this PA.

Discrete Distributions. The discrete distribution used in this report is the Poisson distribution. The Poisson PDF is often used to model the number of events taking place over intervals of time, such as the arrival of telephone calls at a switch station (queuing problem) or the number of imperfections per unit length produced in a bolt of cloth.

Constructed Distributions (Subjective). Constructed distributions of Subjective type are histograms based on subjective estimates of range (the 0 and 100 percentile) and at least one interior percentile point (usually the 50 percentile or median). The subjective estimates of percentile points are usually obtained directly from experts in the subject matter of the parameter of concern. Histogram PDFs for intrinsically continuous parameters are always converted to piecewise linear CDFs by joining the subjective percentile points with straight lines.

Miscellaneous Categories. Other "null" categories of distributions are described below:

Constant. When a distribution type is listed as constant, a distribution has not been assigned and a constant value is used in all PA calculations.

Table. The table category of data indicates that the parameter varies with another property and the result is a tabulated value. For example, relative permeability varies with saturation; its distribution type is listed as table (the median value is not meaningful and is therefore omitted in the table).

4

Probability Density Function f(x)	Cumulative Distribution Function F(x)	Expected Value μ	Variance σ^2
1. Beta			
$\frac{1}{B(\alpha,\lambda)} \frac{(x-a)^{\alpha-1} (b-x)^{\lambda-1}}{(b-a)^{\alpha+\lambda-2}}$ <p>$a < x < b, \alpha > 0, \lambda > 0$</p>	$\int_a^x f(x) \, dx$	$a = \frac{\alpha}{\alpha + \lambda}$	$\frac{(b-a)^2 \alpha \lambda}{(\alpha + \lambda)^2 (\alpha + \lambda + 1)}$
where			
$B(\alpha,\lambda) = \frac{\Gamma(\alpha) \Gamma(\lambda)}{\Gamma(\alpha+\lambda)} \quad \text{and} \quad \Gamma(\gamma) = \int_0^\infty x^{\gamma-1} e^{-x} dx$ <p>$= \frac{\alpha! \lambda!}{(\alpha + \lambda - 1)!}$ if α and λ are integers</p>			
2. Gamma			
$\frac{\lambda^\alpha x^{\alpha-1} e^{-\lambda x}}{\Gamma(\alpha)}$	$\int_a^x f(x) \, dx$	$\frac{\alpha}{\lambda}$	$\frac{\alpha}{\lambda^2}$
3. Exponential			
$\lambda e^{-\lambda x} \quad x \geq 0$	$1 - e^{-\lambda x}$	$\frac{1}{\lambda}$	$\frac{1}{\lambda^2}$

Table 8-1. Description of Several Probability Distributions (Continued)

Probability Density Function f(x)	Cumulative Distribution Function F(x)	Expected Value μ	Variance σ²
4. Normal N(μ, σ²)			
$\frac{1}{\sigma\sqrt{2\pi}} \exp \left[-\frac{(x-\mu)^2}{2\sigma^2} \right]$	$\int_{-\infty}^x f(x) dx$	μ	σ²
$-\infty \leq x \leq \infty$			
but for PA			
$a \leq x \leq b$ where $P(x > a) = 0.99$ and $P(x > b) = 0.01$		$\mu = \frac{a+b}{2}$	$\left(\frac{b-a}{4.66} \right)^2$
5. Lognormal		$\exp \left[\mu(y) + \frac{\sigma^2(y)}{2} \right]$	
$\frac{1}{\sigma x \sqrt{2\pi}} \exp \left[\frac{1}{2\sigma^2} (\ln x - \mu)^2 \right]$	$\int_{-\infty}^x f(x) dx$	Median = $e^{\mu(y)}$	$e^{2\mu(y) + \sigma^2} (e^{\sigma^2(y)} - 1)$
$x \geq 0$			
$x = e^y$ where $y = N(\mu, \sigma^2)$			
but for PA			
$P(y > a) = 0.99$ and $P(y > b) = 0.01$		$\mu(y) = \frac{a+b}{2}$	$\sigma^2(y) = \left(\frac{b-a}{4.66} \right)^2$

Table 8-1. Description of Several Probability Distributions (Continued)

Probability Density Function $f(x)$	Cumulative Distribution Function $F(x)$	Expected Value μ	Variance σ^2
6. Uniform			
$\frac{1}{b-a} \quad a \leq x \leq b$	$\frac{x-a}{b-a}$	$\frac{a+b}{2} = \mu$	$\frac{(b-a)^2}{12}$
7. Loguniform			
$\frac{1}{x(\ln b - \ln a)}$	$\frac{\ln x - \ln a}{\ln b - \ln a}$	$\frac{b-a}{\ln b - \ln a}$	$(b-a) \left[\frac{(\ln b - \ln a)(b+a) - 2(b-a)}{2(\ln b - \ln a)^2} \right]$
8. Poisson (discrete)			
$\frac{\mu^x e^{-\mu}}{x!} \quad x = 0, 1, 2, \dots, \infty$	$\sum_{x=0}^x f(x)$	μ	μ

8.1.2 Some Limitations on Distributions

A major limitation of ensuring valid probability distributions is the lack of an actual disposal site for the INEL spent nuclear fuel and waste. However, other limitations on ensuring the validity of the probability distributions assigned to parameters in the performance assessment are thought to be a consequence of two assumptions that are frequently made in analyses of geologic disposal systems:

- The equating of the variability of a parameter in space (e.g., spatial variation of porosity) with parameter uncertainty, in a model (where the model uses a constant value), particularly for that class of parameters called material-property parameters.
- The neglect of obvious correlations between model parameters (e.g., permeability and porosity).

Current methods of assigning uncertainty to some of the material-property parameters (e.g., including small-scale spatial variability as a source of uncertainty) may distort results of sensitivity analyses, but will probably not affect the relative ranking of the various waste types or the validity of results of the uncertainty analyses that are used to make preliminary comparisons with EPA standards. The following argument attempts to explain the two limitations described above. The following text is taken from Sandia WIPP Project, 1992, Volume 3, Chapter 1.

No Scaling of Variability for Material-Property Parameters. The performance models described in Chapters 9 through 14 of this report are based on the numerical solution of one or more of three types of equations:

- (a) Partial differential equations - which are reduced to a set of algebraic equations or ordinary differential equations in order to effect a solution by finite-difference or finite-element methods. Examples: the equations of groundwater and brine flow, solute transport, and gas flow (see Chapters 12 and 13).
- (b) Ordinary differential equations - which may be the result of a reduction of a partial differential equation or may directly model the dynamics of a lumped-parameter system, e.g., punctured brine reservoirs, leaching and decay of radioactive waste stored in a panel (see Chapter 13, Simplified Consequence Modeling).
- (c) Algebraic equations of the form

$$F(x_1, x_2, x_3, \dots, x_n; y) = 0$$

which may arise indirectly from equilibrium solutions of ordinary differential equations (i.e., solutions for time $\rightarrow \infty$) or may directly express a model of some physical relationship between performance-model variables ($x_1, x_2, x_3, \dots, x_n$) and y , an intermediate dependent variable.

In addition to dependent variables and independent variables of position and time, certain constant quantities appear in each of the three types of equations. In most cases, these parameters are intended to represent physical and chemical properties of real materials of the disposal system: e.g., the hydraulic conductivity, porosity, and specific storage in models of fluid flow. This kind of parameter is called a *material-property parameter* in the remainder of this section.

Several of the material-property parameters of performance models have been included in the set of uncertain variables sampled in this study.

The distribution of a material-property parameter needs to reflect spatial variability of the material property and also the scale of the model. The zones or cells of numerical models (finite-element, finite-difference, or lumped-parameter models) must be few in number to minimize computational time and expense; in a typical problem involving geologic media, these cells will have dimensions of tens of meters or more and volumes of thousands of cubic meters. Material-property parameters must therefore represent the effects of a physical or chemical property of matter in these relatively large, arbitrarily defined volumes of space. It follows that material-property parameters are model dependent and usually not observable quantities, i.e., quantities that can be measured in the field or in the laboratory. On the other hand, with few exceptions most physical and chemical properties of geologic materials are

actually measured on spatial scales typical of the laboratory or an exploratory borehole, a matter of at most a few tens of centimeters, with the possible exception of large-scale pumping tests for evaluating transmissivity. In addition, natural materials and many man-made materials (e.g., defense waste) tend to be inhomogeneous on spatial scales that are smaller than the scales that characterize model cell sizes; accordingly, a set of measurements of a material property taken randomly from large volumes of real material may show wide variability. The question is: How to assign a distribution to material-property parameters in a way that correctly reflects both cell size and the small-scale variability that may appear in measurements of the corresponding material property?

One way of approaching the problem of scaling is as follows. Assume that the material property can be represented as a scalar field in space, say $\phi(x)$, where $x = (x, y, z)$ denotes position in space. (The assumptions of a scalar quantity in three dimensions are for the sake of simplicity of argument and involve no loss of generality; the property could be a vector or tensor.) It is argued in some modern textbooks (e.g., de Marsily, 1986, Chapter 13 and Section 4.4) that the material-property parameter, say Φ , to be used in the numerical solution of the partial differential equation should be taken as a spatial average of ϕ over the cell or zone; for instance, in a cell or zone of volume V ,

$$\Phi(V) = \frac{1}{V} \int_V \phi(x) dx \quad (8-1)$$

where dx is the volume element $dx dy dz$. (Again, no loss of generality is involved; if appropriate, a line or surface average could replace the volume average.)

To account for spatial variability of $\phi(x)$, it can be assumed that ϕ is a *stationary, random scalar field* within a cell volume V , with realizations $\phi(x, \mu)$ and the following statistical properties:

$$\text{Expectation of } \phi(x, \mu) = E[\phi(x)] = \bar{\phi}, \text{ a constant,} \quad (8-2)$$

and

$$\begin{aligned} \text{Covariance of } \phi(x, \mu) &= E\{[\phi(x) - \bar{\phi}][\phi(y) - \bar{\phi}]\} \\ &= \sigma^2 \rho(|x - y|), \end{aligned} \quad (8-3)$$

where σ^2 is a *variance* of ϕ , and $\rho(\cdot)$ is a function of $r = |x - y|$ with the properties,

$$\rho(r) \geq 0 \text{ for } r \in 0, \infty, \quad (8-4)$$

$$\rho(r) \rightarrow 1 \text{ as } r \rightarrow 0,$$

$$\rho(r) \rightarrow 0 \text{ as } r \rightarrow \infty.$$

The function $\rho(\cdot)$ is called the *autocorrelation function* (Yaglom, 1962); it is a measure of the statistical dependence of the values of ϕ measured at two different points x and y . The stationarity assumptions of constant mean value $\bar{\phi}$ and variance σ^2 can be slightly weakened by allowing these quantities to depend on the coordinates of the center of the volume V , i.e., $\bar{\phi}$ and σ^2 may vary from cell to cell.

Treating $\phi(x)$ as a stationary random field with statistical properties 8-2 through 8-4 allows estimates of the mean value and variance of the volume average of ϕ , $\Phi(V)$, to be made. It is shown in textbooks (see for instance Yaglom, 1962, p. 23-24) that

$$\text{Expectation of } \Phi(V) = E[\Phi(V)] = \bar{\phi}, \quad (8-5)$$

and

$$\text{Variance of } \Phi(V) = \frac{\sigma^2}{V^2} \iint_V \rho(|x - y|) dx dy. \quad (8-6)$$

If $\bar{\phi}$, σ^2 and $\rho(r)$ were known, the problem would be essentially solved in that the distribution of the material-property parameter, $\Phi(V)$, could be approximated by a normal distribution with mean and variance given respectively by Eqs. 8-5 and 8-6. In general, $\bar{\phi}$, σ^2 and the function $\rho(r)$ must be estimated using sets of spatially coordinated measurements of the material property ϕ , say $(\phi_1, \phi_2, \dots, \phi_N)$. The estimators of $\bar{\phi}$ and σ^2 are the usual unbiased estimators of mean and variance (see Tierney, 1990, pp. II-4,5) and, given a sufficiently large set of spatially coordinated measurements of ϕ , approximations to the autocorrelation function could be constructed and used in numerical evaluations of the volume integrals in Eq. 8-6. This ideal solution to the problem cannot be implemented, however, since there are few measurements of the material properties for the disposal system models and most are not spatially indexed. Thus, one must try to use available measurements and insight to infer the statistical properties, given by Eqs. 8-5 and 8-6, of material-property parameters, $\Phi(V)$. The following two general observations are useful in inferring statistical properties of material-property parameters.

First, variance of a material-property parameter is less than or equal to the apparent variance of the material property. Note that because of the properties of $\rho(r)$ (Eq. 8-4), the integrand in the double volume integral of Eq. 8-5 is always less than one so that

$$\text{Variance of } \Phi(V) \leq \sigma^2.$$

In particular, if the special form of autocorrelation function is taken ("cookie cutter"),

$$\begin{aligned} \rho(|x-y|) &= 1 \text{ if } |x-y| \leq a, \\ &= 0 \text{ otherwise,} \end{aligned} \quad (8-7)$$

then

$$\text{Variance of } \Phi(V) \approx \frac{v}{V} \sigma^2, \quad (8-8)$$

where $v = \frac{4\pi}{3} a^3$ can be called the *volume of correlation*. Equation 8-8 suggests that if the volume of correlation is $\ll V$, then the distribution of $\Phi(V)$ is peaked about the mean value of the material property, $\bar{\phi}$. If the coefficient of variation of the material property, $\sigma/\bar{\phi}$, is not large (say, of the order of one), the distribution of $\Phi(V)$ is more sharply peaked about the mean value, $\bar{\phi}$, than is the distribution of the material property, $\phi(x)$. If this tendency is strong enough, then $\Phi(V)$ can simply be assigned the mean value,

$$\Phi(V) \approx \bar{\phi}.$$

This is what is usually done in studies with numerical models that are not probabilistic; that is, not directed explicitly towards sensitivity and uncertainty analyses.

Second, if as suggested above, $\Phi(V) \approx \bar{\phi}$, then one must consider the uncertainty inherent in estimating the mean value $\bar{\phi}$, that arises from two sources: (1) a limited number of measurements of the material property, and (2) relationships between $\bar{\phi}$ and other uncertain problem parameters. Uncertainty of the first type can be handled by fitting available data to a "t-distribution" (Blom, 1989) which, in a Bayesian approach, gives the distribution of the true mean of the material property about the sample mean of measurements. However, this was not done in assigning ranges to parameters here. Also, the standard techniques cannot be used when the distribution of the material property, $\phi(x)$, must be gained by subjective means, i.e., the elicitation of expert judgment. In such cases, it is necessary to make the assumption that the distribution of the material property, $\phi(x)$, is also the distribution of the material-property parameter, $\Phi(V)$. Instances where this assumption was made are found in the estimation of radionuclide solubility. Uncertainty of the second type is usually model dependent and must be handled on a case-by-case basis (see remarks on correlations below).

General Absence of Correlation Among Parameters. Most of the 51 parameters varied during the current performance assessment exercise were assumed to be independent random variables even though it was known that some were dependent upon others, i.e., correlated in some way. Correlations of the model variables may arise from

the fact that there are natural correlations between the local quantities used to determine the form of the model variable (e.g., local porosity could be strongly correlated with local permeability); or correlations of model variables may be implicit in the form of the mathematical model in which they are used. The effects of neglecting correlations on the sensitivity/uncertainty analyses are generally unknown.

8.1.3 Parameters Selected for Sampling

A parameter was initially selected as imprecisely known in the 1994 PA if (1) the parameter had proved to be sensitive in the 1993 PA (Rechard, Ed., 1993), or (2) the parameter was thought to be at least moderately sensitive in a new consequence model for this PA. To keep the calculations tractable, this initial list was then reduced to 51 parameters, about half of which were used primarily in gas consumption and source term submodels. These were then separated into two samples of 27 each (with three dummy variables). To help keep the number of sampled parameters to a minimum, we assumed that some hydrologic characteristics of specific layers (i.e., hydraulic conductivity, fracture spacing, Parker-van Genuchten parameter, and sorption coefficients) were 100% correlated. Table 8-3 displays the mapping scheme. The assumed distributions for these 51 parameters are shown in Figures 8-1 through 8-14.

Parameters sampled in the engineered barrier were fraction of fuel with initially failed cladding; alteration rates of waste-immobilizing matrices; alteration rates of layers of the container; solubilities of neptunium, protactinium, plutonium, and uranium; sorption coefficient on rust of container; effective area for diffusion of contaminants; fraction of containers with failed outer layer; and area above container that contributes water for corrosion and transport through the container.

Parameters sampled in the geologic barrier were the Parker-Van Genuchten " β " value for the matrix, bulk hydraulic conductivity, matrix hydraulic conductivity, and fracture spacing for Topopah Spring, Calico Hills, and Prow Pass. The sorption coefficients for neptunium (Np), plutonium (Pu), and uranium (U) in the devitrified and zeolitic tuffs were also sampled. Climate change was simulated by sampling on minimum and maximum infiltration rates and the "wet" cyclic period within 100,000 yr. Also, we sampled a factor that concentrated a portion of infiltration into one element of the two-dimensional mesh. Finally, the borehole diameter for the intrusion borehole and the frequency of intrusion were sampled.

8.1.4 Parameters Held Constant

A total of about 3000 parameters were required by the consequence and probability models for the tuff site. The dimensions of important engineered and geologic features of the site are not considered as part of the total number of parameters.

Because only 51 parameters were varied, the majority of modeling parameters were held constant, usually at the median value. Yet ranges and distributions were estimated for many of these parameters to examine the potential validity of the single value assigned. The tables of the model parameters are presented in Chapters 4, 5, and 6 for the waste parcel, geologic barrier, and repository, respectively. Model parameters for the gas generation and source term submodels are provided in Chapter 11.

Table 8-2. Parameters Varied at Tuff Repository for 1994 Performance Assessment Calculations

Parameter Description ^b					Sampling Variables ^a	
					Flow	Transport
Engineered Barrier						
Waste Parcel						
Waste Form						
1	Fraction of fuel with initially failed cladding	$f_{\text{clad},101}$	WEP101	ECff	USATCONC & GASSNF	1
2		$f_{\text{clad},201}$	WEP201			2
		$f_{\text{clad},102}$	WEP102			
3		$f_{\text{clad},202}$	WEP202			3
		$f_{\text{clad},103}$	WEP103			
		$f_{\text{clad},203}$	WEP203			
4	Alteration rate of layer or matrix of waste parcel	r_{ceramic}	Ceramic	CoR_A_Wo	USATCONC & GASSNF	1
5		r_{glass}	Glass			2
6		r_{UO2}	UO2			3
7	Solubility of radionuclides in J-13 water, without silica saturation	$\log(S_{\text{Np}})$	Np	LogSolM	USATCONC & NUTS	4
8		$\log(S_{\text{Pa}})$	Pa		& STAFF3D	5
9		$\log(S_{\text{Pu}})$	Pu		& TOSPAC	6
10		$\log(S_{\text{U}})$	U			7
11	Solubility of radionuclides in J-13 water, with silica saturation		Np	LogSolMS	USATCONC & NUTS	8
12			Pu		& STAFF3D	9
13			U		& TOSPAC	10
14	Fraction released immediately for matrix 2	$C_{\text{gap},203}$	WEP203	QRF_M2C	USATCONC	11
15		$CS_{\text{gap},203}$	WEP203	QRF_M2Cs		12
16		$I_{\text{gap},203}$	WEP203	QRF_M2I		13
17		$TC_{\text{gap},203}$	WEP203	QRF_M2Tc		14
Waste Container						
18	Alteration rate of layer or matrix of waste parcel	r_{SS304}	SS304LP	CoR_A_Wo	USATCONC & GASSNF	4
19		r_{In825}	IN825			5
20		r_{CST}	CSteel			6
21	Effective area for diffusion	A_{Diff}	Canister	effDArea	USATCONC	15
22	Sorption coefficient on rust ^c of container	Kd_{U}	U	KdFe	USATCONC	16
23		Kd_{Pu}	Pu	KdFe		27
24	Area above container contributing water	A_{C}	Canister	effCArea		26
			dummy	dummy		7
			dummy	dummy		8
			dummy	dummy		9
25	Fraction of containers with failed outer layer	f_{early}	Canister	EBFrac	USATCONC & GASSNF	10
Repository						
26	Fraction of containers with rubble	f_{rubble}	Canister	bacFrac	USATCONC & GASSNF	11
Geologic Engineered Barrier						
Unsaturated Zone						
Hydrologic/Bulk						
27	Hydraulic conductivity of layers	Kb_{Tsw}	Tsw	BlkGas	BRAGFLO_T & STAFF3D	12
28		Kb_{CHnv}	CHnv		& TOSPAC	13
29		Kb_{PPw}	PPw			14

^a Numbers indicate order in which the parameters were sampled.

^b More complete descriptions are provided in Figures 8-1 through 8-14.

^c Although several products would be produced from corrosion of the containers, the only product treated in the 1994 PA is rust from corrosion of the carbon steel disposal container.

Table 8-2. Parameters Varied at Tuff Repository for 1994 Performance Assessment Calculations (Continued)

Parameter Description ^b					Sampling Variables ^a	
					Flow	Transport
Symbol	Material ID	Parameter ID	Computational Model			
Hydrologic/Matrix						
30 Hydraulic conductivity of matrix	K _{TSW}	Tsw	Hycndsam	BRAGFLO_T	15	
31	K _{CHnv}	CHnv		& STAFF3D & TOSPAC	16	
32	K _{PPw}	PPw			17	
33 Van Genuchten “β”	β _{TSW}	TSw	VGBeta	BRAGFLO_T	18	
34	β _{CHnv}	CHnv		& TOSPAC	19	
35	β _{PPw}	PPw			20	
Hydrologic/Fracture						
36 Spacing of fractures	2B _{TSW}	TSw	FracSpac	BRAGFLO_T	21	
37	2B _{CHnv}	CHnv		& STAFF3D	22	
38	2B _{PPw}	PPw		& TOSPAC	23	
Saturated and Unsaturated Zones						
Transport						
39 Sorption coefficients - devitrified tuff	K _{ddNp}	Np	KdD	NUTS	18	
40	K _{ddPu}	Pu		& STAFF3D	17	
41	K _{ddU}	U		& TOSPAC	21	
42 Sorption coefficients - zeolitic tuff	K _{dzNp}	Np	KdZ		20	
43	K _{dzPu}	Pu			22	
44	K _{dzU}	U			19	
45 Dispersivity fraction	α _F	Global	Dispperc	NUTS & STAFF3D	25	
Agents Acting Upon Disposal System						
Climate Change						
46 Base infiltration rate	i _{infil}	Global	PptInfMn	BRAGFLO_T	24	
47 Infiltration amplitude	A _{infil}		PptInfMx	& TOSPAC	25	
48 Period	T _{infil}		CyclePer		26	
49 Infiltration concentration factor	f _{infil}		PptInfOc		27	
Drilling Intrusion						
50 Borehole diameter	D _{bore}	Borehole	Diammod	WPRD	23	
51 Intrusion lambda	λ _{intru}	Global	Lambdag	CCDFPERM	24	

^a Numbers indicate order in which the parameters were sampled.

^b More complete descriptions are provided in Figures 8-1 through 8-14.

^c Although several products would be produced from corrosion of the containers, the only product treated in the 1994 PA is rust from corrosion of the carbon steel disposal container.

^a Numbers indicate order in which the parameters were sampled.

^b More complete descriptions are provided in Figures 8-1 through 8-14.

^c Although several products would be produced from corrosion of the containers, the only product treated in the 1994 PA is rust from corrosion of the carbon steel disposal container.

Table 8-3. Mapping of Sampled Hydrologic Parameters

Hydrologic Modeling Layer*				Hydrologic Parameters**			Transport Parameters (Kd)***		
No.	Symbol	Name	Type	Parker-Van Genuchten	Hydraulic Conductivity	Fracture Spacing	Np	Pu	U
1	TCw	Most of Tiva Canyon	Welded, devitrified	←	3-TSw	→	Kdd	Kdd	Kdd
2	PTn	Paintbrush	Non-welded, vitric	←	5-CHv	→	1/4 Kdd†	Kdd	Kdd
3	TSw	Most of Topopah Spring	Welded, devitrified	←	3-TSw	→	Kdd	Kdd	Kdd
4	TSv	Small portion of Topopah Spring	Welded, vitrophyre	Constant	3-TSw	3-TSw	Constant	Constant	Constant
5	CHnv	Calico Hills/ Prow Pass	Non-welded, vitric	←	5-CHv	→	1/4 Kdd	Kdd	Kdd
6	CHnz	Calico Hills/ Prow Pass	Non-welded, zeolitic	3-TSw	5-CHv	5-CHv	Kdz	Kdz	Kdz
7	PPw	Prow Pass	Welded, devitrified	←	7-PPw	→	Kdd	Kdd	Kdd
8	CFUn	Upper Crater Flats	Non-welded, zeolitic	←	Constant	→	Kdz	Kdz	Kdz
9	BFw	Bullfrog	Welded, devitrified	3-TSw (BRAGFLO_T only)	Constant	3-TSw (BRAGFLO_T only)	Kdd	Kdd	Kdd
10	CFMn	Middle Crater Flats	Non-welded, zeolitic	←	Constant	→	Kdz	Kdz	Kdz
11	TRw	Tram	Welded, devitrified	←	Constant at BFw	→	Kdd	Kdd	Kdd

* The hydrologic modeling layers frequently combine geologic layers that have a hydrologic characteristic in common, such as "welded".

** The number-symbol (e.g., 3-TSw) refers to a modeling layer. For example, 3-TSw in Row 1 indicates that Tiva Canyon (layer 1) and Topopah Spring (layer 3) have identical distributions and values and are 100% correlated.

*** Kdd refers to sorption in devitrified tuff; Kdz refers to sorption in zeolitic tuff. Corresponding Kd's (e.g., Kdd for Np, layers 1 and 2) have identical distributions and values are 100% correlated.

† One-fourth of the devitrified value for neptunium is assigned to the neptunium in vitric tuff.

8. Probability Modeling

TRI-6342-4484-0

Figure 8-1. Probability distributions of fraction of fuel with initially failed cladding. Distributions include fraction of silicon-carbide coatings that have failed in the waste parcels containing graphite spent fuel (WP 101, 201), fraction of fuel from N-Reactor fuel (WP 102, 202), and Shippingport spent fuel (WP 103, 203) with initially failed zircaloy cladding.

TRI-6342-4492-0

Figure 8-2. Probability distributions for alteration rate of layer or matrix of waste parcel. Distributions include alteration rates per surface area (constant in front of exponential term of Arrhenius rate equation) of glass-ceramic matrix-immobilizing calcine high-level waste, borosilicate glass immobilizing high-level waste from all sources, and uranium dioxide (UO₂) in Shippingport and pressurized water reactor fuel.

8. Probability Modeling

Figure 8-3. Probability distributions for solubility of radionuclides in J-13 water without silica saturation. Distributions include neptunium, plutonium, and uranium in J-13 water, without silica saturation, and the probability distribution for protactinium in water with and without silica saturation. The distribution and sampled value for plutonium was also used for americium and samarium. (Distributions from Wilson et al., 1994.)

TRI-6342-4494-0

Figure 8-4. Probability distributions for solubility of neptunium, plutonium, and uranium in J-13 water, with silica saturation. The distribution for plutonium and sampled value was also used for americium and samarium.

8. Probability Modeling

TRI-6342-4495-0

Figure 8-5. Probability distributions for fraction released immediately for matrix. Distributions include fraction of carbon-14 in gap between zircaloy cladding and uranium dioxide, and fraction of cesium-137, iodine-129, and technetium-99 present in grain boundaries of uranium dioxide of the Shippingport and pressurized water reactor fuel, which is released immediately when cladding fails.

TRI-6342-4485-0

Figure 8-6. Uniform probability distributions of alteration rates for layer and matrix of waste parcel. Distributions include alteration rates per surface area (constant in front of exponential term of Arrhenius rate equation) for waste parcel materials: Stainless Steel 304L (in handling container, borated stainless steel fuel supports, and capsules for advanced test reactor fuel), Incoloy Alloy 825 disposal container, and ASTM Type A-516, grade 60, carbon steel.

8. Probability Modeling

TRI-6342-4496-0

Figure 8-7. Probability distributions for sorption coefficient of uranium and plutonium on rust of outer carbon steel disposal container (Wilson et al., 1994); effective area, including tortuosity, for diffusion of radionuclides through the breached containers, and area above container that contributes water (e.g., drips), that in turn contacts the container surface.

TRI-6342-4487-0

Figure 8-8. Probability distributions of fraction of containers with failed outer layer and with direct contact with water in the matrix of the host rock for a significant portion of the 10,000-yr regulatory period (i.e., no time dependence of contact).

8. Probability Modeling

TRI-6342-4488-0

Figure 8-9. Probability distributions of hydraulic conductivity for layers and matrix. Distributions include bulk matrix, saturated hydraulic conductivity assigned to modeling layers Tsw, CHnz, and PPw, CHnv and CHnz, and PPw; and matrix hydraulic conductivity assigned to Tsw, TCw, and CHnz, CHnv and PTn, and PPw (distribution from Wilson et al., 1994).

TRI-6342-4489-0

Figure 8-10. Probability distributions for coefficient " β " in van Genuchten model of two-phase saturation assigned to TSw, TCw, and CHnz modeling layers, CHnv and PTn modeling layers, and PPw modeling layer (distribution from Wilson et al., 1994).

8. Probability Modeling

TRI-6342-4490-0

Figure 8-11. Probability distributions for dispersivity factor (dispersivity factor • travel distance) and for spacing of fractures assigned to modeling layers TSw, TSv, and TSw, CHnv, CHnz, and PTn, and PPw (distributions from Wilson et al., 1994).

8. Probability Modeling

TRI-6342-4491-0

Figure 8-13. Probability distributions for global parameters for climate change. Distributions include infiltration rate above repository for current dry climate, increase in infiltration rate during wet climate, period of climate change, and potential concentration of infiltration because of surface features above the repository. The resulting shape of the function for infiltration is also shown.

Figure 8-14. Probability distributions for global parameters for drilling intrusion: diameter of intrusion borehole and λ for Poisson function of frequency of intrusion into the repository.

8.2 Poisson Model for Probability of Human Intrusion

8.2.1 Probability Model

The probability model of human intrusion by exploratory drilling is based upon the assumption that the number of inadvertent drilling events in a time interval $[a, b]$ follows a homogeneous Poisson process, i.e., the probability $P(n)$ that $n = 0, 1, 2, \dots$ events occur in $[a, b]$ is given by

$$P(n) = \frac{[\lambda(b-a)]^n}{n!} \exp[-\lambda(b-a)],$$

where λ is a constant called the drilling intensity (see Tierney, 1991, Appendix C) (Figure 8-15). In practice,

$$\lambda = A_p \lambda^*$$

where A_p is the total of the projected areas of all containers ($A_p = Na$, N the total number of canisters and a the projected area of a canister on the ground's surface above the repository). The quantity λ^* is a mean drilling rate for which the EPA (1993, Appendix C) has set an upper limit as follows for sites involving nonsedimentary rocks:

$$\lambda_{\max, \text{tuff}}^* = \frac{3 \text{ boreholes}}{10^6 \text{ m}^2 \cdot 10^4 \text{ yr}} = 3 \times 10^{-10} \text{ m}^{-2} \cdot \text{yr}^{-1}$$

For the calculations for the tuff repository, λ^* is uniformly varied between 0 and $\lambda_{\max}^*$.

8.2.2 Area Ratios for Probability of Hitting Different Waste Parcels

To evaluate the complementary cumulative distribution function of releases from a repository filled with different waste waste parcels, the probability of a drillbit hitting a particular waste parcel must be known because the radionuclide content of each waste parcel type varies. In evaluating the probability of a drillbit hitting a specific type of waste parcel, the location of the drilling rig is assumed to be random such that the probability of hitting a waste parcel type, given that a hit has occurred, is the ratio of the cross-sectional area of the waste parcel type to the cross-sectional area of the repository (disposal region of repository).

The probability of a drill bit intersecting a waste parcel is proportional to the "enhanced area" of the drill and the waste parcel (i.e., the maximum area obtainable from the dimensions of the drill and the waste parcel). In the 1994 PA, both vertical and horizontal waste emplacement schemes were considered for the waste disposal group. In addition, the drillbit diameter was sampled, so that the hit probability tables are unique according to the drillbit diameter. The formula for $P(w_g)\text{hit}$, the probability that a intrusion drilling event will hit any waste parcel in the repository, is

$$P(w_g)_{\text{hit}} = \frac{N_1 f(d_1)}{A_{\text{repos}}} + \frac{N_2 f(d_2)}{A_{\text{repos}}} + \dots \quad (8-9)$$

where,

- w_g = the waste disposal group,
- N_i = the number of i th type waste parcels in the waste disposal group,
- $f(d_i)$ = the enhanced areas of intersection of the drill bit and the waste parcel, and
- A_{Repos} = the area of the repository.

b)

$$P \{N=n\} = \frac{(\lambda t)^n}{n!} e^{-\lambda t}$$

Poisson Analytic Probability Model

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Figure 8-15. Probability of a human-intrusion estimated by Poisson analytic probability model with constant λ .

8. Probability Modeling

In this analysis, the A_{Repos} was assumed to be the area of the disposal region.

For vertical emplacement, two different geometric waste parcel areal projections exist: square (LWT) and circular (DOE standard containers). The borehole emplacement of the LWT containers results in a horizontal projection area, $f(d_i)$, of the drill and the i th type of waste parcel as

$$\pi(r_{\text{drill}})^2 + (s_{\text{LWT}})^2,$$

where r_{drill} is the drillbit radius and s_{LWT} is the side length of the square LWT container. Similarly, for the vertical emplacement of the cylindrically shaped DOE standard container, the horizontal projection area, $f(d_i)$, of the drill and the i th type of waste parcel is

$$\pi((r_{\text{drill}})^2 + (r_{\text{PARCEL}})^2),$$

where r_{PARCEL} is the radius of the i th type of waste parcel.

For horizontal in-drift emplacement of the MPCs, the horizontal projection area, $f(d_i)$, of the drill and the i th type of waste parcel is

$$(L_{\text{PARCEL}} + d_{\text{drill}})(d_{\text{PARCEL}} + d_{\text{drill}}),$$

where d_{drill} is the drill diameter, L_{PARCEL} is the length of the i th type of waste parcel, and d_{PARCEL} is the diameter of the i th type of waste parcel.

The ratios for both the horizontal and vertical waste emplacement schemes are presented for one sampled drillbit diameter in Table 8-4.

8.3 Summary of Modeling Assumptions for Human Intrusion

- Human intrusion from drilling follows a homogeneous Poisson process with constant expectation for each simulation.

8.4 A Note on the Fault Tree Formation

The probability of a criticality event in the repository was estimated in this study by means of a fault tree formation (see Appendix B). More precisely, a fault tree was used to calculate an intensity function (events/yr) for a top event "repository criticality," in terms of the probability-per-year of about 30 "basic" events, including events such as drilling through repository, repository flooding and volcanism. The estimated intensity function for all types of repository criticality, 1.6×10^{-6} per year, was then used in a Poisson model to calculate a probability of at least one criticality event in 10,000 yr. The elemental probability of at least one event in 10,000 yr (1.6×10^{-2}) is combined in Chapter 7 with elemental probabilities of other significant events to form the probabilities of the eight summary scenarios considered in the present study.

No background on fault-tree formalism and notation is given in Appendix B. Good explanations of these methods can be found in Apostolakis (1974), Barlow and Lambert (1975), or in the original manual for the SETS code (Worrell and Stack, 1978).

Table 8-4. Probabilities of Hitting a Particular Type of Waste Parcel for One Sampled Drillbit Diameter*

Waste Parcel ID No.	Probability of Hit**	Waste Factor	Waste Parcel Description
Horizontal			
101	0.0074	0.01200	Graphite Spent Nuclear Fuel (SNF)
102	0.0053	2.11330	N-Reactor (Hanford) SNF
103	0.0228	0.12400	Shippingport SNF
104	0.0029	0.05490	Highly enriched uranium Advanced Test Reactor SNF
105	0.0035	0.16200	Low enriched uranium commercial pressurized water reactor SNF
106	0.1301	0.32000	INEL calcine glass-ceramic high-level waste
107	0.0844	8.03600	Savannah borosilicate glass, high-level waste
108	0.0313	1.16000	Hanford borosilicate glass, high-level waste
109	0.0044	0.07150	West Valley borosilicate glass, high-level waste
No Hit:	0.7080		
Vertical			
201	0.0010	0.01200	Graphite SNF
202	0.0007	2.11330	N-Reactor (Hanford) SNF
203	0.0027	0.12400	Shippingport SNF
204	0.0004	0.05490	Highly enriched uranium Advanced Test Reactor SNF
205	0.0004	0.16200	Low enriched uranium commercial pressurized water reactor SNF
206	0.0189	0.32000	INEL calcine glass-ceramic high-level waste
207	0.0123	8.03600	Savannah borosilicate glass, high-level waste
208	0.0046	1.16000	Hanford borosilicate glass, high-level waste
209	0.0006	0.07150	West Valley borosilicate glass, high-level waste
No Hit:	0.9584		

* The probabilities are based on a borehole diameter of 0.0508 m. When the borehole diameter is sampled, each vector has its own table of hit probabilities.

** Although the use of more than two significant digits may indicate a certainty beyond what is considered reasonable, we have maintained the form digits so that data output in subsequent calculations could be traced back to its original form in tables such as this.

9. Modeling Drilling into Repository (CUTTINGS)

J. S. Rath

9.1 Background

Of the possible events that can influence the quantity of radionuclides reaching the accessible environment, one of the most important for a repository is that caused by the inadvertent penetration of the disposal region by exploratory drilling.* Such drilling can create a pathway that over time allows radionuclides to be released through groundwater flow; in fact, the consequence models for a salt repository are concerned solely with this pathway. However, exploratory drilling can also cause an immediate release of radionuclides through the cuttings, cavings, or spillings brought to the surface in the drilling fluid (mud). Thus, the cuttings pathway can be a significant pathway in terms of release limits set by 40 CFR 191.† Although the cuttings pathway is less significant when releases are calculated in terms of individual dose rate, the cuttings calculations are included here for completeness.

The significance of release from cuttings depends upon the drilling frequency assumed (see Chapter 8, Probability Modeling). The discussion in Chapter 15 indicates those CCDFs for which releases from cuttings were included. A description of the cuttings model and its results are provided below.

9.2 Description of Drilling Mechanisms

The 1994 PA assumes that future drilling techniques will be similar to today's techniques for exploration of hydrocarbons and other economic minerals (the same assumption was used in the 1993 PA). The specific drilling technique assumed is rotary drilling with liquid in which a cutting bit is attached to a series of hollow drill pipes that is rotated and directed downward. To remove the material loosened by the drilling action, a drilling fluid ("mud") is pumped down the drill pipe, through and around the drill bit, and back up to the surface within the annulus formed by the drill pipe and borehole wall.

In a tuff repository, two mechanisms can influence the quantity of radionuclides brought to the surface when a container is inadvertently penetrated by an exploratory drillhole. The first mechanism is caused by the cutting action of the drill bit, which removes a volume of waste (cuttings) equal to the product of the drill bit area times the repository thickness. The second mechanism is erosion of the borehole wall (cavings) adjacent to the waste caused by the flowing drilling fluid. A third mechanism (spalling) can also occur in an area with near-lithostatic pressures from gas generated by corrosion, but these large pressures are not possible in the porous tuff venting to the atmosphere.

9.3 Description of Model

For this performance assessment (and in the 1993 PA), any hit on a container is assumed to remove the original but decayed contents of a container to the drilling mud pit and the surface; in essence, no material is assumed to dif-

* The guidance in Appendix B; 40 CFR 191, suggests that exploratory drilling into the repository is the most severe type of inadvertent intrusion that must be considered.

† The cuttings/cavings pathway has been studied in performance assessments for the WIPP Project since 1990 (e.g., Bertram-Howery et al., 1990; WIPP PA Division, 1991a; WIPP PA Dept., 1992a) because it represents a possible path for moving a quantity of radionuclides to the surface. The cuttings/cavings calculations were run originally as scoping calculations in response to an attempt to identify "energy sources" that could move a quantity of waste sufficient to violate the standard from the repository horizon to the land surface (WIPP PA Group, 1990). A plausible energy source was drilling fluid in an exploratory drilling operation. The bounding calculation helped to answer the question, "on average, how many containers can be released before a violation occurs?" The pathway continues to be of interest for compliance with 40 CFR 191 because of the quantity of radionuclides brought to the surface, even though 40 CFR 191 neglects direct release as a pathway (except for ^{14}C , which uses atmospheric release) and instead conservatively bounds direct release by using the pathway to humans from drinking surface water (EPA, 1985b; O'Brien et al., 1977).

9. Modeling Drilling into Repository (CUTTINGS)

1 fuse out of the waste parcel in 10,000 yr. For consistency with this assumption, no radionuclides are removed when
2 the canister is missed. In actuality, after corrosion of the waste parcel, a plume of dissolved radionuclides would be
3 transported from the waste parcel by advection and diffusion. Although this phenomenon is modeled in the ground-
4 water flow situation, the increase in accuracy that would be enabled here is expected to be insignificant and thus did
5 not warrant the difficulty of coupling the evaluation of the plume with the cuttings calculations. Hence the model
6 includes only equations that calculate the decay of the original inventory to the time of intrusion.
7

8
9 For the 1994 PA, the computer code WPRD, Waste Parcel Radioisotope Decay, was developed. WPRD consid-
10 ers times of intrusion (Figure 9-1 and Appendix F) and probabilities of using different drill bit diameters and hitting a
11 horizontal MPC or vertical LWT containing various waste types (Table 9-1). These results are combined by means of
12 CCDFPERM (see Chapter 7 and Appendix G) with the probability of intrusion (Chapter 8) to form a CCDF of the
13 cuttings releases.
14
15

16 All 63 radionuclides from the initial inventory listed in Chapter 4 and Appendix A are considered in the WPRD
17 code; these are the same radionuclides considered in the source-term submodel (Chapter 11). The abbreviated chains
18 for radioactive decay were also used in the cuttings computation (see Figure 4-8 in Chapter 4).
19
20

21 The inventory includes anticipated waste to be emplaced in the year 2030 and is based on currently existing
22 waste or waste that will be generated from minimal treatment of currently existing spent fuel. The actual release to
23 the ground surface is governed by the spacing of the waste parcels in the repository (Chapter 6), the type of waste par-
24 cel (Chapter 4), the probability of intrusion (Chapter 8), the probability of hitting various waste parcels based on the
25 cross-sectional area (Chapter 8), and the drillbit diameter, which was a sampled parameter (Chapter 8).
26
27

28 For the drillbit diameter, a discrete distribution of 14 common drillbit sizes with equal probability was used. The
29 sizes ranged from 0.05 m (2 in.) to 0.61 m (2 ft). The maximum drillbit diameter of 0.61 m (2 ft) was used as a con-
30 stant value in TSPA-1993 (Wilson et al., 1994, p. 16-3). The use of this drillbit size assumes that the operator is
31 searching for natural gas at a target elevation of 6000 m (~19,500 ft) in sedimentary rocks underlying the repository.[‡]
32 It should be noted, however, that little evidence of hydrocarbons exists in the area. A more likely situation would be
33 an exploratory drillhole for hard rock economic minerals such as zeolites for sorption material (e.g., kitty litter) and
34 silica for silicon. These drillholes would be small and would not penetrate much beyond 300 m (1000 ft), so that
35 those drillholes that did reach the repository would be near their target elevation. Based on this situation, a bit diam-
36 eter of 0.05 m (2 in.) was selected as the minimum diameter.
37
38
39
40
41

9.4 Intermediate Results

42 As noted in Chapter 7 (Scenario Development), six time intervals (100-150; 150-200; 200-500; 500-1500; 1500-
43 4500; and 4500-10,000 yr) were used to discretize the 10,000-yr regulatory period for calculating releases through
44 drill cuttings. Drilling intrusions were assumed to occur at the midpoints of each of the six time intervals, i.e., 125,
45 175, 350, 1000, 3000, and 7250 yr. Releases through groundwater, however, were calculated using only a single
46 intrusion at 1000 yr. For comparison, Figures 9-1 through 9-22 show the initial and potential activity release in curies
47 from cuttings of each of the 22 waste parcels (11 per waste emplacement scheme) at the 1000-yr intrusion. The
48 potential activity release for all six time intervals is tabulated in Appendix F.
49
50
51
52
53

54 A comparison of the radioactive decay within each of the 22 waste parcels is shown in Figure 9-23. Generally,
55 activity in a waste parcel decreases by factors of 100 to 1000 during the first 1000 yr. The radionuclides that are most
56 important to the total activity at 1000 yr can be evaluated from Figures 9-1 through 9-22 (and, for other times, from
57 the tables in Appendix F).
58
59
60
61

62 [‡] Although large drillbit sizes have recently been used for exploratory drilling to reach deep targets, a counter trend is to decrease the size to
63 decrease costs. For example, techniques such as "thin wire" drilling and "closed loop" drilling are being used for deep sea drilling in the North
64 Sea to reduce the volume of drilling fluids and cuttings. These techniques may find favor in the United States for reducing environmental dam-
65 age from large mud bits. Hence, "current" drilling practices 5 to 10 years from now may lead to a large reduction in the amount of direct release
66 from inadvertent intrusion.

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Figure 9-1. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP101, graphite spent fuel in Multi-Purpose Canister.

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Figure 9-2. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP102, N-Reactor spent fuel in Multi-Purpose Canister.

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Figure 9-3. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP103, Shippingport spent fuel in Multi-Purpose Canister.

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Figure 9-4. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP104, highly enriched spent fuel in Multi-Purpose Canister.

Figure 9-5. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP105, low enriched spent fuel in Multi-Purpose Canister.

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Figure 9-6. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP106, calcine high-level waste from INEL in glass ceramic in four DOE standard canisters placed in Multi-Purpose Canister.

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Figure 9-7. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP107, high-level waste from Savannah River in four DOE standard canisters placed in Multi-Purpose Canister.

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Figure 9-8. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP108, high-level waste from Hanford in four DOE standard canisters placed in Multi-Purpose Canister.

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Figure 9-9. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP109, high-level waste from West Valley in four DOE standard canisters placed in Multi-Purpose Canister.

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Figure 9-10. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP110, caliche high-level waste from INEL as borosilicate glass placed in four DOE standard canisters and placed in a Multi-Purpose Canister (Simple PA only).

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Figure 9-11. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP111, calcine high-level waste from INEL packaged loose in four DOE standard canisters and placed in a Multi-Purpose Canister (Simple PA only).

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Figure 9-12. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP201, graphite spent fuel in a Legal Weight Truck container.

Figure 9-13. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP202, N-Reactor spent fuel in a Legal Weight Truck container.

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Figure 9-14. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP203, Shippingport spent fuel in a Legal Weight Truck container.

Figure 9-15. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP204, highly enriched spent fuel in a Legal Weight Truck container.

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Figure 9-16. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP205, low enriched spent fuel in a Legal Weight Truck container.

TRI-6342-4437-0

Figure 9-17. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP206, calcine high-level waste from INEL as glass ceramic in DOE standard canister.

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Figure 9-18. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP207, high-level waste from Savannah River in DOE standard canister.

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Figure 9-19. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP208, high-level waste from Hanford in a DOE standard canister.

9. Modeling Drilling into Repository (CUTTINGS)

Figure 9-20. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WPP209, high-level waste from West Valley in a DOE standard canister.

Figure 9-21. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP210, calcine high-level waste from INEL as borosilicate glass in a DOE standard canister (Simple PA only).

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9. Modeling Drilling into Repository (CUTTINGS)

TRI-6342-4442-0

Figure 9-22. Initial (year 2030) and potential activity per package of 63 radionuclides considered in the performance assessment for WP211, calcine high-level waste from INEL packaged loose in a DOE standard canister (Simple PA only).

(a)

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(b)

Figure 9-23. Total curie content per package at six intrusion times for (a) horizontally emplaced waste parcels of spent fuel (WP101 to WP105), (b) vertically emplaced waste parcels of spent fuel (WP201 to WP205), (c) horizontally emplaced waste parcels of high-level waste (WP106 to WP111), and (d) vertically emplaced waste parcels of high-level waste (WP206-WP211).

9. Modeling Drilling into Repository (CUTTINGS)

(c)

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(d)

Figure 9-23. Total curie content per package at six intrusion times for (a) horizontally emplaced waste parcels of spent fuel (WP101 to WP105), (b) vertically emplaced waste parcels of spent fuel (WP201 to WP205), (c) horizontally emplaced waste parcels of high-level waste (WP106 to WP111), and (d) vertically emplaced waste parcels of high-level waste (WP206-WP211) (continued).

9.5 Summary of Modeling Assumptions for Cuttings Removal

- Future drilling techniques during 10,000-yr regulatory period are the same as today.
- Drilling that hits a container removes entire original but decayed contents of a container to the surface.
- Drilling that misses a container removes no radionuclides.
- Boreholes are vertical.
- Activity of abbreviated decay chains for 63 radionuclides from inventory are accurate enough to evaluate release.
- From Latin Hypercube sampling, the drill bit diameter mean is 0.29545 m, the median is 0.26512 m, and the range is 0.0508 to 0.6096 m. (Delta distribution is used.)

10. Criticality Modeling

L. C. Sanchez, R. P. Rechard, D. R. Evans, P. J. Sentieri, and J. R. Wilson

A self-sustaining nuclear chain reaction (critical condition) can occur when a sufficient amount of fissile isotopes (e.g., ^{233}U , ^{235}U , ^{239}Pu , and ^{241}Pu) come together in a specific concentration, or density, and shape of certain temperatures, and most preferably with a specific amount of neutron moderator (e.g., water). Sufficient fissile isotopes are present in the 125-ton multi-purpose canister for both the low and highly enriched spent fuel. The highly enriched spent fuel, however, easily meets the concentration criterion under most conditions. This experimental highly enriched fuel usually had little fissioning of the ^{235}U , so its "burnup" is low.* Although the waste container design proposed in this report is intended to maintain subcritical conditions with an appropriate margin of safety, even when flooded with water, through the use of borated stainless steel, water may enter the repository and alter the waste and containers through corrosion. Therefore, the probability and consequences of a critical mass of fissile material assembling from spent fuel under conditions that would allow a self-sustaining nuclear chain reaction must be examined.

One approach to reducing criticality concerns would be to require extensive treatments, such as (1) limiting mass of fissile material per container, (2) removing all fissile material from the spent fuel and then storing this material in a location other than the repository, or (3) chemically altering the fuel and then diluting it with depleted or natural uranium. These options, which were considered as part of the 1993 PA, could reduce the probability of a criticality to near zero. In contrast, the 1994 PA explored direct waste disposal without special treatment to determine the probability of a criticality occurring under these conditions and, if one occurred, the nature of the consequences. Note that the use of borated stainless steel is modeled in the 1994 PA, which can be considered as a prudent, though less certain, means of criticality control than the options mentioned above.

The first section describes the various analytical approaches used in the 1994 PA. The remainder of the chapter provides information about these approaches. The basic conditions under which a criticality can occur are reviewed in Section 10.1.2. Four specific situations from the event tree that could lead to a self-sustaining nuclear chain reaction are outlined in Section 10.2. Various options that could be used to diminish the probability of a critical event are discussed in Section 10.3. Section 10.4 discusses work that guided later detailed analysis; pertinent aspects of scenario development and probability modeling, including the fault tree, are briefly mentioned here (see also Chapters 7 and 8). Although the probability of occurrence for one of the criticality scenarios from the event tree cannot be easily dismissed, simple bounding calculations reveal small consequences, as fully described in Appendix B. Sections 10.5 and 10.6 describe the detailed analysis, including results, of phenomena that either lead up to a criticality or would be operating during a criticality. (The results are also summarized in Chapter 15 and the Executive Summary.) Section 10.5 presents processes leading up to a critical event. These results can be used in gaining an understanding of the probability of a critical event occurring. Section 10.6 presents processes that operate during the criticality, along with some mathematical models and associated descriptions. A summary of the findings from the 1994 PA, is provided in Section 10.7, along with recommendations on future work.

10.1 Analysis Approach and Terminology

This section describes the various analytical approaches used to explore the consequences of a criticality. The section also briefly introduces basic concepts and terminology necessary to understand these approaches, which may be helpful to readers unfamiliar with nuclear physics.

* Although the issue of criticality could be important for low enriched commercial fuel, the probability of occurrence is lower and so a study of these conditions did not rank high in priority as highly enriched fuels.

10.1.1 Approach to the Analysis

As in any modeling effort, the approach to analyzing critical conditions began with the gathering of data. An important aspect for developing a preliminary event tree was the review of past critical events in nature and those induced by humans. After this preliminary work, Sandia and LITCO each assumed specific tasks of the criticality analysis to explore quickly the various approaches within the time allotted (Figure 10-1). Even with a division of tasks, however, it was not possible to explore all aspects of the probability and consequences of a criticality in or near a repository. The aspects studied in the 1994 PA were those that were judged to be most important for the program (for example, only horizontally emplaced multi-purpose canisters were evaluated) and/or computationally tractable (for example, development and simulation with a fully coupled nuclear dynamics and thermal-fluid flow code were not attempted).

Within the analyses performed by Sandia and LITCO, three different types of models were used for criticality modeling. These models investigated the consequences of critical assemblies in situ and the neutronic coupling of adjacent waste containers. The first model is a refinement of the work performed in the 1993 PA on the minimum spacing necessary to eliminate neutronic coupling (the cross-talk interactions of neutrons) between adjacent containers. The second model attempted to bound the incremental increase in the inventory of fission products and the magnitude of the additional thermal energy in the repository due to criticality excursions by assuming a reactor at steady state for 10,000 yr. Estimated bounds from this model were compared to data from past criticality accidents. The third model examined the energy releases from a repository assuming a dynamic situation including processes that would stop the reaction, such as lack of water.

As discussed in Chapter 2, current regulations lack guidance regarding either the technical acceptability of an occurrence of a critical condition or the type of calculations that would be acceptable to a regulator to show that a reasonable effort had been made to calculate the probability and consequences of a critical event. In response to this void, the 1994 PA used a variety of calculations that approach the problem from different viewpoints. The calculations are intended to demonstrate to the technical community the possible approaches for bounding or, alternatively, approximating either the probability or consequences of a critical event in a geologic repository in tuff. These calculations can thus (1) form the basis of rational decisions on policy concerning criticality in a repository and (2) serve as the basis for a procedure, a methodology, or a style of calculations for examining criticality in a repository.

10.1.2 Concepts of Criticality and Related Terminology

To appreciate the likelihood of a criticality occurring in an underground repository of radioactive waste, it is important to understand the concept of a critical condition. The following is a discussion of basic principles of a nuclear chain reaction based upon the discussion in Harper (1961, p. 5-9) for readers who are not familiar with nuclear physics.

Nuclear Chain Reaction. In a fission reaction (splitting of atoms), more neutrons are emitted than are required to start it. If loss of neutrons is not too great, a chain-reaction can build up. Loss of neutrons takes two forms: sorption of neutrons without the production of fission and loss of neutrons from the system (Figure 10-2). The latter is very important because neutrons go through solid matter like water through a sieve. In a small piece of fissile material, one stray neutron will not start a chain reaction, even if absorbed by a fissionable isotope, because the neutrons emitted by the fission nearly all escape before starting another fission. In a larger piece of fissionable material, neutrons would have less chance of escape, and in an infinite block they could never escape (they could only be lost to sorption by elements that do not fission). With no loss of neutrons at all, and more than one neutron liberated per fission, the rate of fission increases until a change in physical conditions imposes a limit.

Multiplication Factor. In a large block of fissile material (such as ^{235}U), some of the original neutrons will produce second-generation neutrons, some third, a few fourth, and so on. Ultimately, allowing for all the generations, there may be many more fissions produced than neutrons originally present, but if each generation contains fewer neutrons than the preceding one, there will be a limit to the total number. To be precise, if n neutrons are introduced

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Figure 10-1. Sequence of work performed and interfaces between different approaches for evaluating probability and consequences of criticality in a large, horizontally emplaced, multi-purpose canister in a tuff disposal system for 1994 PA.

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Figure 10-2. Simple schematic of fission chain reaction showing three generations of neutrons from fission of ^{235}U . To simplify the diagram, it has been assumed that each fission results in the formation of two fission fragments and three neutrons. The neutrons released as the nucleus fissions are "prompt" neutrons. Neutrons released from a few of the fission fragments are "delayed" neutrons. Although the delayed neutrons represent only about 0.7% of the neutron population, they are very important in reactor dynamic analysis (after Duderstadt and Hamilton, 1976).

into the block initially, and there are kn in the second generation, there will be k^2n in the third, k^3n in the fourth, and so on. In all, the total number of neutrons that would appear in the block due to n initial neutrons is given by

$$\text{total number of neutrons that would appear in block} = n \sum_{r=0}^{\infty} k^r \quad (10-1)$$

If $k < 1$, the sum converges and is equal to $n/(1 - k)$.

If we can measure the neutron population in one neutron generation and again in the next generation, then the ratio of these numbers would be the multiplication factor k . (In real systems, it is the effective multiplication factor, most commonly denoted as k_{eff}):

$$\text{Multiplication factor } (k_{\text{eff}}) = \frac{\text{Number of neutrons in one generation}}{\text{Number of neutrons in preceding generation}} \quad (10-2)$$

Because the number of fission neutrons in any generation is proportional to the number of fissions during each generation, then k_{eff} corresponds to the ratio of fissions from generation to generation (and hence power level ratio). If the reactor (or assembly of fissionable fuel) has the right configuration and composition so that the number of neutrons always remains the same, then $k_{\text{eff}} = 1$ (the system is referred to as being "critical"). The three possible situations are:

Table 10-1. Multiplication Factor

$k_{\text{eff}} < 1$	subcritical (zero or decreasing power)
$k_{\text{eff}} = 1$	critical (could be at any power level)
$k_{\text{eff}} > 1$	supercritical (increasing power)

Nuclear processes occur very quickly, thus the generations succeed each other swiftly. Unless k_{eff} is nearly equal to unity, the first few terms in the series contribute most of the sum (see Equation 10-1), and the corresponding generations of neutrons are born and die in a short interval of time. If the multiplication factor k_{eff} is less than but not too close to 1.0, spontaneous fissions in the block will give rise to more fissions, but the total number will remain fairly small. Each spontaneous fission, and each arrival of a stray cosmic-ray neutron, will provoke activity.

If the block were just that size for which $k_{\text{eff}} = 1$, any neutron present will, after death, leave exactly one survivor, and so on through the generations (assuming no additional neutron source). Thus any population of neutrons that happens to be present survives indefinitely, the number of neutrons remains constant, and the rate of fission continues unchanged. The block is said to be critical, and in this condition, remains in a steady state irrespective of the size of the population of neutrons. If fissile material is removed from the block, or k_{eff} becomes less than unity for any other reason (see section, Feedback to Arrest Critical Conditions), the size of the population of neutrons cannot be maintained by the reproduction of neutrons and the population falls to the low value associated with stray neutrons; in the absence of stray neutrons it would fall to zero. In either case, the reaction stops.

If more fissile material is added so that $k_{\text{eff}} > 1$, any activity already present, however small, can multiply indefinitely (Figure 10-2). As the interval between generations is small, the multiplication is rapid and the activity can rise rapidly to tremendous values. In such circumstances, however, the resultant liberation of heat quickly expands or breaks apart the supercritical mass, reducing k_{eff} below unity, and stopping the reaction before all the fissile material can be used up (see section on Feedback to Arrest Critical Conditions). A major explosion results if the neutron population increases significantly before the expansion of the fissile material, but this condition is extremely difficult to achieve and there is no credible scenario in a geologic repository that would yield this situation. It requires a supercritical mass to be assembled so rapidly that there is insufficient time for an expansion or minor explosion to occur during assembly when k_{eff} only slightly exceeds unity. In a fission bomb, it is necessary to bring the components of the supercritical mass together with literally explosive force, something that cannot happen by accident.

Reflection and Moderation to Promote Critical Conditions. In reactor design, materials are frequently placed around a nuclear reactor core containing the fissile materials to reflect back into the core many of the neutrons that would otherwise escape. Common reflector materials, which may also be moderators, in a nuclear reactor are graphite, beryllium, water, and natural or depleted uranium. Materials (moderators) are also used directly in the reactor core to promote critical conditions by slowing down the high-velocity neutrons from the fission process since slow (thermal) neutrons have a much greater probability of producing a fission in fissile material. Common moderators in a nuclear reactor are natural ("light") water, "heavy" water (water with significant quantities of the deuterium isotope) and graphite because they slow down neutrons effectively while absorbing few of them.

Feedback to Arrest Critical Conditions. During a supercritical excursion, the power and temperature will rise until negative feedback becomes large enough to reduce the multiplication effects to a subcritical condition. The most important negative feedback from temperature are (1) density decrease (which is important for metal systems, in which the neutron leakage from the assembly is increased), (2) Doppler effects (since broadening of resonance cross sections of the non-fissile material may be important to the reduction of the neutron multiplication), (3) thermal expansion with or without boiling (which is a major feedback mechanism for dissolved systems), and (4) desaturation of groundwater. If supercriticality cannot be counteracted by these negative feedback effects, the assembly breaks apart or melts (for metal assemblies) or disassembles by boiling (solutions). As will be argued for the 1994 PA, the most likely criticality event would be one that corresponds to a feedback mechanism of boiling of the water moderator from within the remains of the waste container or a nearby fissile material precipitation zone. This is a very effective negative feedback mechanism since a natural reactor within tuff would likely be at atmospheric pressure and not pressurized.

10.2 Repository Conditions with Potential for a Criticality

This section describes two basic events leading up to a self-sustaining nuclear chain reaction in or near a container (i.e., a criticality).[†] The two basic events, which are used to form an event tree with four different situations, are (1) sufficient or insufficient water to efficiently moderate a nuclear chain reaction and (2) fast or slow assembly of the mass of fissile material (Figure 10-3). Examples of all four situations follow, together with a review of natural analogues, and criticality experiments and accidents that are relevant to a criticality in a repository.

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Figure 10-3. Event tree with two basic events—availability of water and rate of assembling a critical mass—that result in four basic types of self-sustaining nuclear chain reactions. Several processes are necessary to lead up to these events (see Section 10.5). These events are folded into the base case (see Chapter 7).

Although examples are presented for all four outcomes, the probability that they could occur within a repository varies substantially. Two methods were used to develop an understanding about the likelihood of the four outcomes. One method was to develop a fault tree in which several distinct events leading up to a critical condition were postulated, and the corresponding probabilities of occurrence for each event were properly combined to arrive at overall probabilities. The second method was to model relevant phenomena such as dissolution of uranium and boron, corrosion of containers, and precipitation of isotopes, and then observe whether conditions conducive to a self-sustained nuclear chain reaction occurred. These approaches are described in Sections 10.4 and 10.5, respectively.

Table 10-2 provides more details about situations that could result in a criticality chain-reaction. As can be seen in this table, the five excursion situations can be analyzed in one of three ways: (1) fast nuclear system disassembly, which can be analyzed by the Bethe-Tait method, (2) thermal/solution disassembly, which is characterized by existing data on criticality accidents in processing plants, and (3) thermal non-disassembly, which is analyzed as an Oklo-type phenomenon. A discussion of the possible scenarios follows. The critical event studied in the 1994 PA most closely resembles Scenarios E3E4 (see Figure 10-3).

[†] Although these events are part of scenario development, specific aspects of the criticality in a repository are discussed here to provide sufficient background for those readers who wish to concentrate on the criticality calculations only instead of the performance assessment as a whole.

10.2.1 High Moderation, Slow Assembly (Oklo Natural Reactors)

Scenario E3E4 (Figure 10-3 and Table 10-2) corresponds to very slow chemical changes in which, after the waste container had been corroded, the fissile fuel or the neutron absorber material is dissolved, the generated solution is transported away from the container location and (in the case of the fissile material) precipitates out. It may be possible to avoid the scenario by the use of engineered controls (use of soluble neutron absorber in designs). Yet, in either case, the equations describing the physics are the same as identified later in this chapter.

Table 10-2. Nuclear Criticality Possibilities in a Geologic Repository*

Location	Undisturbed**				Human Intrusion
	Insitu Near/Far Field	Insitu Near Field			Non-Insitu
Scenario	Very slow assembly from chemical change with water moderation, E3E4	Very slow assembly from chemical change with water moderation, E3E4	Fast assembly without water for moderation, E3E4	Slow assembly without water for moderation, E4	Fast assembly with water for moderation, E3
Description*	Corrosion of container, dissolution of fissile material and precipitation in near/far-field location	Corrosion of container, dissolution of neutron absorber and transport of neutron absorbers away from container	Sudden movement of fissile material or neutron absorbers due to earthquake, structural failure, etc.	Slow crumbling of waste and collection at bottom of container	Brought to surface, moderated with drilling mud or surface water
Type of reactor assembly	Thermal reactor	Thermal reactor	Fast reactor	Breeder reactor	Thermal reactor
Type of criticality analysis	Oklo	Oklo	Bethe-Tait	Bethe-Tait	Bethe-Tait and Table 10-3

* These situations do not take into account the possible design features of a waste container. See Section 10.4 and Appendix B for complete fault tree.

** A dry, critical silica-moderated system was not analyzed because mechanisms for forming such a system appeared implausible.

The time history of k_{eff} and the power for the fission system is expected to be similar to that shown in Figure 10-4. It may be expected that the precipitation zone (nuclear assembly) would be generated very slowly over time (times scales may on the order of thousands to tens of thousands of years or more). The system would be subcritical for a long period of time and gradually rise to a criticality constant value near unity (say 0.99998) and slowly increase to unity. The system would be expected to very slightly exceed unity (say 1.00001) and the system power would rise. Likewise, the temperature for the system core region would also rise. However, when the system temperature rises, the system criticality constant would decrease and become subcritical because of temperature feedback[‡] effects such as (1) density change of the water moderator (slight decreases in the density of the moderator could be enough to change the criticality constant from 1.00001 to a subcritical value and stop the generation of power), (2) boiling of the moderator (significant power generation would cause the moderator to leave the core region of the nuclear assembly

[‡] In addition to negative feedback from temperature increase, numerous fission products (materials produced as fission occurs) are strong neutron absorbers, especially ¹⁴⁹Sm and a number of other rare-earth elements, and can reduce reactivity. As time passes, they build up to a level where power is decreased until equilibrium is reached. Fissile material depletion also would reduce power. However, the low power associated with the high moderation-slow assembly scenario probably makes these two power limitation mechanisms negligible.

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Figure 10-4. Hypothesized time history for temperature, power output, and multiplication factor for highly moderated, slow-assembly critical events. An asymptotic approach to long-term critical excursion is possible, but the analysis would require a fully coupled set of nuclear dynamics codes.

and would change the system to a subcritical configuration), and (3) temperature increases in the fissile material would result in the "Doppler" effect (the broadening of resonance cross sections for sorption of neutrons "without fission").

After substantial time has elapsed during which thermal-hydraulic phenomena have lowered the system to near ambient thermal conditions, the cycle of criticality, power and temperature increase followed by criticality, power and temperature decrease might be repeated (see Figure 10-4). This type of behavior has occurred in nature in the past when the concentration of ^{235}U was sufficient and is known as the "Oklo phenomena" after the Oklo site in the country of Gabon in West Africa.

Sixteen different natural reactors have been identified in the Oklo uranium deposit in Gabon, Africa. In the early 1970s, French scientists determined that uranium ore taken from localized regions at that site had ^{235}U isotope concentrations that were half the typical amount (0.7 weight percent of the uranium). Other isotopes that resembled those of spent fuel generated by nuclear power plants were also identified. This and other site information indicated that Oklo was at one time a natural reactor. The date at which it operated has been placed at about 1.7 to 2.0 billion years ago. The period of operation has been estimated from 500,000 yr to 800,000 yr, and the temperature of operation is thought to have ranged from 410 to 725 K, which corresponds to a pressurized water reactor. About 1.7 to 2.0 billion years ago, the natural uranium had an enrichment in ^{235}U that was about 3 weight percent of the uranium, which was high enough, under appropriate conditions, to create a critical assembly. (Because ^{235}U has a shorter half-life than ^{238}U , natural uranium presently has an enrichment of only 0.72 weight percent, which is not sufficient to allow an Oklo phenomenon to be repeated.) The ore operated as an underground nuclear reactor in which water under pressure percolated down through fractures in the rock and served as a moderator for the assembly. The natural reactor operated in a cyclic manner in which (1) the assembly would become critical only when sufficient water (moderator) was present, (2) the power generated from the nuclear reaction would heat the assembly, (3) at elevated temperatures the water (moderator) would turn into steam, (4) the loss of moderator would shut down the nuclear chain (heat generating mechanism), and (5) over time enough cooling water would re-enter the system to start the cycle over again. This reactor behavior continued for about one million years until the burnup of ^{235}U no longer allowed a critical assembly to form. It is this type of transient nuclear behavior that is thought to be most likely to yield a criticality excursion in a repository.

Although several references exist on the dynamics of the Oklo phenomenon, they do not include any information on the coupling of the neutron transport with the thermal-hydraulics and thus are not useful for this performance assessment (Bilanovic and Harms, 1985; Kuroda, 1990; Cowan et al., 1975; Harms, 1988; Naudet, 1978). The Oklo deposit has been completely mined out. Only assay samples remain, which allow scientists to determine the spatial distribution of radionuclides, but are not helpful in generating a realistic dynamic model.

10.2.2 High Moderation, Fast Assembly (Critical Events in Aqueous Solutions)

Scenario E3 corresponds to fuel assemblies that are essentially flooded. Their behavior would be somewhat similar to that of a critical aqueous type accident (i.e., ^{235}U or ^{239}Pu aqueous solution). Data on several criticality accidents that have occurred in process plants are shown in Table 10-3. This type of criticality excursion could be the result of a human intrusion situation that generates a slurry consisting of fissile material and water (moderator). In the resulting excursion, the slurry would probably go rapidly into a delayed critical (criticality caused by both prompt and delayed neutrons) and then into a supercritical geometry. The rapid heating would cause the moderator to disassemble by splashing or boiling. Also, the high moderation, fast assembly criticality is similar to the SNAPTRAN experiments, which were characterized by fairly large reactivity insertions ($k_{\text{eff}} > 1$). These events were considered to be large criticalities, up to 4×10^{19} fissions (Stratton, 1989). Data regarding accidents involving moderated metal and oxide systems are shown in Table 10-4.

Table 10-3. Criticality Accidents in Processing Plants*

Date	Plant	Total Fissions	Prompt Fissions	Doses (Rads)	Cause
6/16/58	Y-12	1.3×10^{18}	7×10^{16}	365, 339, 327, 270, 236, 69, 69, and 23	^{235}U solution washed into drum
12/30/58	LASL	1.5×10^{17}	1.5×10^{17}	4400 (fatal), 135, and 3	Plutonium concentrated in solvent layer
10/16/59	ICPP	4×10^{19}	10^{17}	50 and 32 (primarily beta)	^{235}U solution siphoned into tank
1/25/61	ICPP	6×10^{17}	6×10^{17}	None	^{235}U solution forced into cylinder by air
4/7/62	Hanford Recuplex	8.2×10^{17}	10^{16}	87, 33, and 16	Plutonium solution in sump sucked into tank
7/24/64	Wood River Junction	1.3×10^{17}	10^{17}	10,000 (fatal), Two 60 to 100	^{235}U solution poured into tank
8/24/70	Windscale	10^{15}	10^{15}	Negligible	Plutonium concentrated in trapped solution
10/17/78	ICPP	3×10^{18}	Unknown	None	^{235}U buildup due to diluted scrub solution

* Taken from Knief (1985), original reference, Paxton (1980). (Data values shown here are in good agreement with those in Stratton, 1989).

In any case, the number of fissions generated in this event may be expected to be on the order of these presented in Tables 10-3 or 10-4 for various accidents involving either the aqueous metals in water solutions or accidents that have occurred in the past. From Table 10-3, it can be seen that the largest excursion identified was 4×10^{19} total fissions (note that the maximum number of immediate fissions is only 6×10^{17}). The number of fissions can be converted into equivalent energy values using the information in Table 10-5. As can be seen, approximately 195 MeV of useful energy (neglecting neutrinos) is released per fission of ^{235}U .

Table 10-4. Criticality Accidents Involving Moderated Metal and Oxide Systems*

Date	Plant	Total Fissions	Prompt Fissions	Doses (Rads)	Cause
6/06/45	LASL	4×10^{16}	3×10^{15}	66, 66, and 7.4	Water leaked into assembly
1950	Chalk River	Unknown	NA	NA	Excess moderator added
6/02/52	ANL	1.22×10^{17}	NA	136, 127, 60, and 9	Control removed, water not removed
12/12/52	Chalk River	1.2×10^{20}	NA	low	Positive void coefficient
7/22/54	INEL	4.68×10^{18}	NA	NA	Planned transient extended
10/15/58	Vinca Yugoslavia	2.6×10^{18}	NA	205, 320, 410, 415, 422, and 433	Faulty power monitoring
3/15/60	Saclay France	3×10^{18}	NA	NA	Removal of absorber rod
1/03/61	INEL	4.4×10^{18}	NA	3 fatalities	Removal of control rod
11/05/62	INEL	1×10^{18}	NA	NA	Planned transient exceeded
12/30/65	Mol Belgium	4.3×10^{17}	NA	NA	Misoperation plus not draining tank
9/23/83	Buenos Aires Argentina	4×10^{17}	NA	low	Failure to drain tank

* Data from Stratton, 1989.

Table 10-5. Useful Energy Released from Thermal Fission of ^{235}U and ^{239}Pu (a)

Fission Product	^{235}U (MeV)	^{239}Pu (MeV)
Light fragments (b)	99.8 ± 1	101.8 ± 1
Heavy fragments (b)	68.4 ± 0.7	73.2 ± 0.7
Fission neutrons (c)	4.8	5.8
Prompt γ -energy	7.5 (d)	~7
β -decay of fission products	7.8 (e)	~8
γ -decay of fission products	6.8 (d)	~6.2 (d)
Total fission energy	195 (f)	202

(a) Source - This table taken from Keepin (1965). ^{239}Pu values are also shown for comparison.

(b) Original source, Milton, 1962.

(c) Energy obtained by multiplying the thermal ν -bar by the average energy (~2 MeV) of fission neutrons.

(d) Original sources, Carver, 1960; Peelle et al., 1962.

(e) Original sources, Armbruster and Meister, 1962.

(f) For simplicity, a value of 200 MeV is often used for the total fission energy.

Table 10-6 was generated using this conversion factor along with other unit conversion factors. From this table it can be seen that the maximum expected integrated total energy release is ~1250 MJ and the maximum quick release of energy is ~19 MJ. It is also noted that the maximum expected integrated total energy release is equivalent to about 0.0145 MWd for all the fuel in that assembly. Also with respect to the immediate energy release, only 19 MJ energy release would be available. This small amount of energy release would be unlikely to cause any significant damage to the immediate rock zone.

Table 10-6. Energy Equivalents for Excursion Fissions (Aqueous)

	Fissions (a)	MJ (b)	kW-hr (c)	MWd (c)	²³⁵ U Burnup (mg) (d)
Total Integrated Fissions	4×10^{19}	1250	347	0.0145	15.6
Prompt Fissions	6×10^{17}	18.7	5.21	2.17×10^{-4}	0.234

(a) Maximum value taken from Table 10-3 (see Knief, 1985, and Paxton, 1980, for original data).
 (b) Calculated from useful energy released value specified in Table 10-5.
 (c) See Appendix H.
 (d) Assuming 1 mg burnup = 22.24 kW-hr.

10.2.3 Low Moderation, Slow Assembly

The low moderation-slow assembly rate Scenario E4 (Figure 10-3 and Table 10-2) can be viewed in the context of the fast breeder reactor. Moderator temperature and void reactivity feedback mechanisms are absent, but fuel temperature and fuel density reactivity feedbacks are sufficient to give stable reactor operations. This type of criticality in a repository would likely have many characteristics in common with the high moderation-slow reactivity insertion case, including power, described in Section 10.2.1.

10.2.4 Low Moderation, Fast Assembly (Experiments with Fissionable Metals)

Scenario E3E4 corresponds to fuel assemblies that contain little or no water or any other moderating materials, i.e., elements such as hydrogen, carbon, and beryllium, which have a high probability of scattering neutrons (because they thermalize/reduce neutron energy) while simultaneously having a low probability of absorbing neutrons. Although this situation appears very improbable, it is discussed here for completeness. This situation would create a "hard" critical nuclear assembly; the "hard" descriptor identifies that the neutrons in this nuclear assembly have a "hard" (high energy) spectrum. Generating a shape that corresponds to this situation is difficult to attain and could only be possible under extremely unusual circumstances. It might require (1) that an earthquake fault somehow breaks up a waste container in such a manner that the fissile material is concentrated together while the neutron absorber (neutron control elements) is simultaneously removed, or (2) that a human intrusion (drilling or mining activities) causes a similar situation (see Table 10-2). The rapid withdrawal of neutron absorbers and/or high concentrations of fissile material would yield a prompt criticality (critical condition with "prompt" neutrons, delayed neutrons not needed) where the power level of the assembly grows at an astronomical rate until the assembly breaks up or vaporizes. Note that even this excursion would not be a nuclear explosion; an explosion would require special design features to enable the generation of massive numbers of fissions and energy release and could not happen by accident. The analysis method for the fast burst excursion is a "Bethe-Tait" type. It should be observed that the Bethe-Tait estimated energy releases for two fast reactors, see Table 10-7, were on the order of 3×10^{19} fissions, even for these large mass assemblies.

Table 10-7. Bethe-Tait Calculations for Fast Reactors (Prompt Fissions)

					²³⁵ U
	Fissions	MJ (a)	kW-hr (b)	MWd (b)	Burnup (mg) (c)
Fermi & EBR-II reactors (d)	3.2×10^{19}	1000	278	0.001157	12.5
850 kg U (50% ²³⁵ U) (e)	2.1×10^{19}	669	186	0.0077	8.09

(a) Calculated from useful energy released value specified in Table 10-5.
 (b) See Appendix H.
 (c) Assuming 1 mg burnup = 22.24 kW-hr.
 (d) Energy values calculated using Bethe-Tait method (Bethe, 1956).
 (e) Energy values calculated using modified Bethe-Tait method (Meyer, 1967).

Also, experiments and accidents at Los Alamos National Laboratory, especially the Godiva reactor, are representative of the low moderation-fast reactivity insertion criticality. Some of the accidents were quite energetic, with fission yields ranging from 10^{16} to 12×10^{17} fissions. Shutdown mechanisms included disassembly, thermal expansion, and, in few cases, melting of the fissile material.

10.3 Potential Techniques to Reduce Probability of Criticality

In a repository, many processes must occur in and around the container before a self-sustaining nuclear chain reaction can take place. Three basic processes that are precursors to establishing critical conditions in a container are (1) sufficient fissionable mass concentration, (2) sufficient water to corrode the container in 10,000 yr (the assumed regulatory period),** and (3) sufficient water to remove any elements near the fissile material that readily absorb neutrons or to provide for dissolution, migration, and then precipitation of the fissile material into a region lacking elements that readily absorb neutrons. (In Figure 7-1 these three precursor processes were collapsed into the base case.)

These three basic processes or conditions are also necessary for sustaining the nuclear chain reaction. Hence, critical conditions within and around the repository—or at least the waste container—either can be prevented or the probability can be greatly reduced by disrupting the processes and conditions. Eight general techniques to disrupt these processes, several of which were studied in either the 1993 or 1994 PAs, are reviewed here. The three methods used in the 1994 PA to determine the probability or consequence of a critical condition in or near a waste container—use of long-lived disposal containers, use of neutron absorbers, and spacing of vertical containers to avoid neutron interactions—are described in Sections 10.3.5, 10.3.6, and 10.3.7.

10.3.1 Storage of Spent Fuel in a Separate Location

Placing the spent nuclear fuel indefinitely in a Monitored Retrieval Storage (MRS) facility would preclude a repository criticality in the DOE-owned spent fuel. Separate storage would also allow future generations the option of recycling the spent fuel. However, the hazards normally associated with fuel storage would be incurred with this alternative. Furthermore, low enriched commercial fuel is susceptible to many of the same criticality issues as highly enriched fuel, although the probability of a criticality occurrence may be lower. This separate storage alternative is beyond the scope of this report and not discussed further.

** Although it would be informative to consider post-regulatory periods, it was beyond the scope of the 1994 PA.

10.3.2 Dilution or Removal of Fissile Mass

Dilution or removal of fissile mass through extensive treatment or reprocessing precludes a criticality in or near the repository from the DOE-owned spent fuel. Possibly, these alternatives could be used in conjunction with the disposal or reuse of fissile material from either weapons dismantlement (NAS, 1994) or the purchase of Russian uranium fuel. These alternatives were considered in the 1993 PA as treatment options; they provided consistent improvement in the performance of the granite and salt disposal systems, in addition to precluding the possibility of criticality. They were not considered further in the 1994 PA.

Dilution. Dilution with depleted uranium or natural uranium could reduce the concentration of fissile ^{235}U to below 1% such that a criticality could not occur when moderated by natural ("light") water. Dilution would increase the volume for some of the highly enriched fuels by a factor of $180^{\dagger\dagger}$ and thus would require a large number of waste parcels, which in turn would enlarge the size of the repository (see Rechard, Ed., 1993). It would also likely be necessary to convert the uranium in the spent fuel and the depleted uranium to the same chemical form rather than perform a simple physical mixing. Conversion would preclude differential dissolution of the various isotopes of uranium but would require facilities similar to those for the removal methods mentioned below. The measure of protection provided by only physical mixing of depleted uranium with spent fuel would have to be examined in future performance assessments.

Removal. Reprocessing the spent fuel to remove fissile material has been done successfully for years at INEL, Hanford, and Savannah River, but involves economic costs. Furthermore, the recovered fissile material would require extensive safeguards, unless it were reused as reactor fuel. Reuse is possibly an economically viable option for ^{235}U , but it is not a clear option for plutonium in the United States at this time.

10.3.3 Limitation of Fissile Mass in Each Waste Parcel

Limiting the mass of fissile isotopes in each waste container ensures that no criticality will occur as long as the fissile isotopes do not dissolve in the groundwater, migrate, and then precipitate elsewhere. Because the amount of water in a tuff disposal system is limited and the saturation of the water with silica is unfavorable to dissolution of uranium, this technique may approach the very low probability associated with the first two alternatives for controlling the possibility of establishing critical conditions. However, as shown in the 1993 PA (Rechard, Ed., 1993), this technique requires a large number of waste containers. Because some highly enriched uranium fuel has an enrichment of 93% ^{235}U , the mass limit is about 0.76 kg ^{235}U , conservatively assuming an optimum sphere moderated by water.

Calculations related to the process of dissolving the uranium and precipitation into pores of the tuff apply to this alternative and are discussed in Section 10.5.

10.3.4 Capability to Drive Water Away from the Repository

Because the presence of water contributes to conditions conducive to a criticality, heating the host rock, which removes water, is a possible means of preventing a criticality. This "hot-repository" concept, which involves tightly packing waste parcels containing many spent fuel assemblies, is being considered by the Yucca Mountain Project for commercial spent fuel disposal. The primary heat source is from ^{90}Sr and ^{137}Cs , which rapidly decay and are essentially eliminated after about 600 yr. The actual length of time that the repository will be hot enough to boil away any water percolating into the repository is uncertain, but this approach to criticality control will eventually cease to be effective. Also, at temperatures above 220°C, aluminum-clad fuel, which forms a significant fraction of the DOE-owned and foreign research reactor inventories, may melt, and above 115°C, highly sorptive zeolites in the tuffs may

^{††} The basis for the volume factor of 180 is dilution with depleted uranium with 0.4% ^{235}U to a final ^{235}U concentration of 0.7%. Diluting to 1% ^{235}U using super-depleted uranium, such as recovered uranium from Savannah River site (~0.2% ^{235}U) reduces the volume increase somewhat.

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be altered and lose their sorptive capability. The possibility of driving water away from the repository was examined in the 1994 PA, and the results are reviewed below.

10.3.5 Use of Long-Lived Disposal Containers

Using corrosion resistant material and corrosion-allowance material in the disposal containers that serve as over-packs for the stainless steel handling container can protect the fissile isotopes and neutron absorber from water dissolution and material relocation for a prolonged period of time. The disadvantage of this approach to criticality control is that the containers would still eventually fail. However, the length of time may be sufficient to meet regulatory requirements. To evaluate compliance with waste package requirements in 10 CFR 60, a high-integrity waste parcel was used in a few of the calculations for both the 1993 PA and the 1994 PA. The length of time to failure of these high-integrity disposal containers was over 10,000 yr if temperature in the repository remains below 60°C. Failure times of less robust containers (disposal containers without a 20-mm layer of Incoloy Alloy 825 or when repository temperatures exceed 60°C) are discussed in Section 10.5.1.

10.3.6 Use of Neutron Absorbers

Placing neutron absorbers in the waste parcels allows more fissile isotopes and, therefore, fewer parcels and still precludes the possibility of a criticality, at least for a time. This technique was assumed in the 1994 PA to allow the option of loading highly enriched spent nuclear fuel into the large handling containers under water. However, if the groundwater were to dissolve the neutron absorbers preferentially, the package contents could become critical. Also, if the fissile material dissolves preferentially, it can migrate and precipitate at a nearby location with no absorber and form a critical mass. The results from the source-term submodel (Chapter 11) that were analyzed to assess the likelihood of these two situations are reviewed in Section 10.5.

10.3.7 Spacing the Containers to Avoid Interactions

Avoiding significant interaction of neutrons between adjacent containers (neutronic coupling) was a criterion used for designing the hypothetical granite and salt repositories in 1993 and the hypothetical tuff repository in 1994. The 1994 calculations refined the 1993 calculations for emplacement of waste containers in vertical boreholes and extended the work to horizontal, in-drift emplacement. A summary of these calculations follows.

In the 1994 PA, a refined analysis of the work initiated in 1993 for neutronic coupling was performed. This model was used to identify the criticality contribution that results from containers being placed near each other. In this configuration, some neutrons are expected to leak (escape) from a waste parcel and then can enter an adjacent waste parcel, thus becoming part of its neutron population. This cross talk interaction of neutrons (neutronic coupling) may be significant enough to require either a minimum separation distance or the insertion of backfill to serve as neutron absorbers between containers. Results indicated that coupling is negligible between vertical oriented waste parcels spaced more than 2 m apart, and negligible for the horizontally oriented waste parcels spaced end to end (see Appendix E for additional discussion).

Note that results obtained with the Monte Carlo code (MCNP) used for the analyses had sizable estimated standard deviations, and the difference between the estimated k_{eff} values were less than the estimated standard deviations (see Appendix E for tabulated computational results). These results occurred because of the excellent neutron-shielding capabilities of the containers. Also, to achieve neutronic coupling, a neutron would have to travel through two shielding walls, i.e., both the container that it is leaving and the container that it is entering.

10.4 Bounding Calculations

10.4.1 Development of a Fault Tree for Repository Criticality

Fault trees have traditionally been used to evaluate the probability of failures within complex human-engineered systems. Using them to evaluate changes in states of components within a geologic repository is possible but requires care. The advantage of fault trees is that this structured approach can quickly identify events and situations that lead to a criticality in a repository. It was this advantage that prompted their use in order to develop hypotheses of behavior. A disadvantage is that the primary components of a tree are usually poorly understood natural processes. Evaluating probabilities for these processes is difficult because while their probability of occurrence may be high, whether they will induce adverse conditions and promote release of radionuclides is not known. Thus, the hypothesized behavior within the fault tree has been examined in more detail and is described in Section 10.5.

The fault tree, developed by Lockheed Idaho Technologies Company, Inc. (LITCO), is fully described in Appendix B. What follows is a brief summary.

Types of Events. The situations in the fault tree start with initiating events that could lead to each of the four types of criticality shown in Figure 10-3. Because the proposed design for the multi-purpose canister assumed in this report includes the use of a borated stainless support structure, the separation of the boron and the spent fuel is very important in determining whether a criticality occurs. Thus, the important event is the removal of boron from the container. (A basic tenet of the fault tree was that the release rate of boron was greater than fissile material; to complement this tenet, the complex phenomena that would contribute to the opposite situation, i.e., uranium being released from the container faster than boron, were also examined and are discussed in Sections 10.5 and 10.6.) Once boron is removed, various types of criticalities are feasible. Note, however, that as shown in the fault tree, a moderated slow assembly (Scenario E3E4) is the most likely.

A criticality at a site far from the waste container was assumed much less probable than a criticality in or near the container. Movement of uranium far from the site would likely involve dispersal of the concentrated fissile material over a much larger area than the waste container. This fissile material would then require some reconcentration. A criticality on the surface, caused by drilling into a waste container, was not considered primarily because the deposition of the fissile material on the surface already represented a release. Also, the criticality was assumed to occur at atmospheric pressure because the container would be breached.

Mechanisms that might cause positive feedback once a critical condition began were dismissed because conditions necessary to assemble a critical mass and continue operation of a nuclear chain reaction were already of a low probability. Further, creating conditions initially that would produce a critical condition reduce the probability even further. For instance, the startup of a nuclear chain reaction in the presence of boronated water was not perceived as possible, so removing the positive feedback gained from removing the boronated water was of no consequence. Likewise, moderation of the chain reaction with silica, which has a positive thermal coefficient of expansion, would require water (simple diffusion of the fissile material into the tuff would not occur within a reasonable time scale) to create the optimal mixture of the fissile material with the silica; hence, the initial conditions would favor startup of the nuclear chain reaction with water as the moderator instead.

Probabilities within Fault Tree. The only credible manner of removing the boron from around the spent fuel was through leaching by water. Hence, the probability of events and processes involved with water leaching primarily determined the computed probability of a criticality event from the fault tree. The primary initiating event influencing the final probability of the fault tree is percolation of water from infiltration of precipitation at the surface. The importance of this phenomenon is similar to that noted for general release of radionuclides disposed of in the repository without a critical event. Possible sources for this water are included in the fault tree, such as increased rainfall at the site due to climate change percolating down a weep that intersects the repository. The probability of these initiating events and the ability of the water to effectively breach the waste is unknown or in dispute. Because the probabilities within the fault tree do not substantially modify the probabilities assumed for the sources of water, the probability remains uncertain. However, the specific value is not as important as the fact that a value of less than

10. Criticality Modeling

10⁻⁴ over 10,000 yr cannot be demonstrated. Such a low value would have eliminated a critical event from further consideration according to the guidance of 40 CFR 191.

Based on the fact that a probability less than 10⁻⁴ over 10,000 yr was not obtained from the fault tree initially produced for the 1994 PA, a significant effort was made to explore both the underlying processes leading up to a criticality and possible consequences from a criticality. The bounding consequence calculations are discussed in the next section (10.4.2). This step was then followed by a more detailed examination of the processes leading up to a criticality and the consequences of the criticality, which are described in Sections 10.5 and 10.6. For example, a factor possibly diminishing the importance of the water percolation flux is that the water is saturated with silica and could potentially lower solubilities of radionuclides; geochemical modeling was done to evaluate this influence.

10.4.2 Steady State Reactor for Evaluating Consequences of High Moderation, Slow Assembly

Consumption of a Portion of Fissile Uranium. Calculations attempted to bound the incremental increase of the fission product inventory and the magnitude of potential energy released in the repository by assuming a reactor at steady state for 10,000 yr. To start this type of calculation, 100% consumption (burnup) of approximately 18% (170 kg) of fissile uranium, ²³⁵U, in one of the 289 MPC containers holding highly enriched uranium was assumed within 10,000 yr. This simple calculation results in about 4.4×10^{26} fissions over 10,000 yr (~44 kW steady-state power).

Limiting Heat Generation to 1 kW Steady State. This value is considered conservative because not only do commercial nuclear reactors achieve typical burnups of only 10 to 20% but they also must dissipate heat to maintain the fuel in optimum configuration and ensure that the water remains liquid so that it is available to moderate the reaction (container is assumed full of water). A simple refinement to the above calculation is to assume that because water is essential for moderating the nuclear reaction (water slows down neutrons so that they have a much higher probability of being absorbed by the ²³⁵U), a limiting case would be a steady-state temperature just below boiling for water in the container. This case corresponds to 950 W or about 1 kW. This power level would consume 1 mg of ²³⁵U per day, or 3.65 kg during 10,000 yr. This consumption rate corresponds to 2.6×10^{18} fissions per day (at 200 MeV per fission), or 9.4×10^{24} fissions over 10,000 yr for a single container (Appendix B).

10.4.3 Increased Fission Product Inventory

The radionuclide inventory in the repository is an important ingredient to the performance assessment. To assess the impact of criticality, it is necessary to calculate the added radionuclides generated by it.

Calculation Method. To provide an upper bound to the radionuclide generation, it was assumed that one canister would go critical soon after repository closure and that sufficient water moderator would be present for 10,000 yr. As discussed earlier, the power level would be about 950 W.

The added radionuclides for the low-power criticality were calculated using the ORIGEN2 computer program, based on the characteristics of a single end-of-life Shippingport fuel element. To obtain the increment in radionuclide inventory resulting from the fission process, the radioisotopes at time zero were allowed to decay for 10,000 yr. The inventory after 10,000 yr of radionuclide decay was subtracted from that corresponding to 10,000 yr of fission. These results were then normalized to the total radionuclide inventory and are shown in Table 10-8 for selected radioisotopes.

As expected, only ²³⁵U and ²³⁸U decreased during the fission process. Fission products, activation products, actinide daughter products, and uranium transmutation products all increased during this period.

Table 10-8. Normalized Increment in Radionuclide Inventory due to 10,000-Yr Fission in Shippingport Fuel Element (from Appendix B)

Radioisotope	Radioisotope Inventory	
	Increment (Ci)	Fraction of Total
$^{14}\text{C}^{(a)}$	6.893×10^{-2}	1.764×10^{-8}
^{90}Sr	3.918×10^5	6.746×10^{-7}
^{90}Y	3.931×10^5	6.766×10^{-7}
^{99}Tc	1.244×10^4	7.796×10^{-5}
^{126}Sn	3.923×10^2	7.654×10^{-5}
^{129}I	2.233×10^1	9.138×10^{-5}
^{135}Cs	1.442×10^3	7.435×10^{-4}
^{137}Cs	4.277×10^5	6.663×10^{-7}
$^{137\text{m}}\text{Ba}$	4.046×10^5	6.683×10^{-7}
^{226}Ra	3.031×10^1	$8.856 \times 10^{-1(b)}$
^{230}Th	5.097×10^1	4.517×10^{-3}
^{232}Th	9.958×10^{-5}	3.831×10^{-9}
^{233}U	7.923	3.597×10^{-7}
^{234}U	1.642×10^3	1.094×10^{-4}
^{235}U	-8.898×10^1	-5.209×10^{-5}
^{236}U	4.178×10^2	7.092×10^{-5}
^{238}U	-5.352×10^{-1}	-7.234×10^{-8}
^{237}Np	7.267×10^2	1.974×10^{-4}
^{238}Pu	1.133×10^5	1.243×10^{-5}
^{239}Pu	1.773×10^4	2.109×10^{-6}
^{240}Pu	3.631×10^4	3.257×10^{-5}
^{242}Pu	1.806	4.625×10^{-7}
^{241}Am	3.793×10^4	4.483×10^{-6}
^{243}Am	1.238×10^2	3.609×10^{-6}

(a) Only from the fission process; Shippingport ORIGEN2 calculations did not consider activation of ^{14}N or ^{13}C , which would increase the inventory by about 4 orders of magnitude.

(b) The production of ^{226}Ra is largely due to the decay of ^{238}Pu , which is produced by neutron activation of ^{238}U .

Gaseous Krypton-85. The ORIGEN2 run was also used to estimate the inventory of gaseous fission products. Of the gaseous fission products, only ^{85}Kr has a long enough half-life (10.73 yr) to accumulate in significant amounts. Because this radionuclide decays more rapidly than it is formed in the high moderated, slow assembly criticality, the total ^{85}Kr inventory in the repository diminishes monotonically as the fission proceeds. Table 10-9 presents the ^{85}Kr inventory at time zero and at 1, 10, 100, 1,000, and 10,000 yr.

Table 10-9. Inventory of ^{85}Kr as a Function of Length of Fission Time Period

Length of Fission (yr)	Inventory of ^{85}Kr (Ci)
0	5.379×10^2
1	5.043×10^2
10	2.828×10^2
100	2.978
1000	2.111
10000	1.979

The worst case for short-lived gaseous fission products such as ^{85}Kr is clearly a short fission process. Therefore, the limiting value for gaseous fission product inventory is no fission at all. Thus, to be conservative, the value at time zero was used in gaseous fission product migration calculations.

Gaseous Carbon-14. The ^{14}C inventory, as gaseous CO_2 , has a long enough half-life (5730 yr) to persist in significant quantities throughout 10,000 yr. Therefore, ^{14}C is of special concern for performance assessment calculations. The following are three potential sources of ^{14}C :

1. Neutron activation of ^{14}N , followed by a proton emission.
2. Neutron activation of ^{13}C .
3. The fission process.

Of these, the principal source is neutron activation [(n,p) reaction] of ^{14}N , which is present in nuclear fuel (and, to a lesser extent, in metals such as zircaloy) as an impurity (Benedict et al., 1981). The small amount of neutron activation of ^{13}C can be predicted since the cross-section seen by a neutron for ^{14}N sorption is 1.87 barn, whereas the cross-section for ^{13}C neutron capture [(n,p) thermal] is 0.9 m barn. Furthermore, for a typical commercial PWR fuel, the fission yield of ^{14}C is approximately four orders of magnitude smaller than the activation yield (Croff and Alexander, 1980). Therefore, for ^{14}C inventories to be correct, it is necessary that the nitrogen impurity present in the fuel be considered in the ORIGEN2 calculations. All the spent fuels probably contain nitrogen impurity, although data were available only for N-Reactor fuel and commercial fuel when the ^{14}C inventory was calculated. However, these two spent fuels represent 90% of the total MTHM of the spent fuel inventory.

The data for low-power fission reported in Table 10-8 are based on ORIGEN2 calculations that do not consider nitrogen impurity, so they do not correctly estimate the ^{14}C increment due to the low-power fission. An approximate value for ^{14}C inventory fractional increment is 1.764×10^{-4} for the 10,000-yr fission. (This estimate is based on the above-cited four-order-of-magnitude ratio of activation ^{14}C to fission product ^{14}C for commercial fuel.)

10.4.4 Repository Effects Due to Increased Fission Product Inventory and Heat

Negligible Effects from Increased Fission Product Inventory. As shown in the previous section, an increase in the fission products from one critical event of 10^{18} fissions is small. The size of the increase is particularly small when compared with the inventory in the repository as follows, which uses the number of fissions as a unit of com-

parison. The assumed size of the repository for the 1994 PA was 12,060 MTHM. Assuming this represents fuel with an average burnup of between 25,000 and 40,000 MWd/MTHM, the number of fissions that is represented by the spent fuel is on the order of 10^{30} , or 12 orders of magnitude greater than one critical event of 10^{18} fissions. Similarly, the 10^{25} atoms split from a critical condition occurring in one container, assuming a steady-state reactor operating for 10,000 yr, is still negligible in comparison to the 10^{30} fissions. Even if one assumes that the 289 waste parcels containing highly enriched spent fuel all go critical, the total fissions of about 10^{28} are only 1% of the inventory represented as fissions.

Negligible Effects from Increased Heat. The amount of heat generated by 1kW steady-state power level over 10,000 yr or 10^{25} fissions over 10,000 yr is minor and no change in the transport properties of the radionuclides would be observed. For example, 1 kW represents a temperature rise of only about 100°C in a perfectly insulated (no heat loss) block of fully saturated tuff the size of the repository over 10,000 yr, based on the data of Table 10-10 and Table H-13 (Volume 3) (i.e., $\Delta T = (10^{25} \text{ fission}) (3.12 \times 10^{-11} \text{ J/fission}) / [(\phi S_w \rho_{\text{water}} C_{p,\text{water}} + (1 - \phi) \rho_{\text{tuff}} C_{p,\text{tuff}})] V$).

Table 10-10. Properties of Tuff and Water for Estimating Temperature Rise in Perfectly Insulated Block of Fully Saturated Tuff

Specific heat of water ($C_{p,\text{water}}$)	4184 J/kg°C
Specific heat of tuff ($C_{p,\text{tuff}}$)	858.3 J/kg°C
Tuff porosity (ϕ)	13.9%
Water saturation (S_w)	100%
Density of water (ρ_{water})	1000 kg/m ³
Density of tuff (ρ_{tuff})	2485 kg/m ³
Volume of repository (V)	$1.1 \times 10^6 \text{ m}^3$

10.5 Process Modeling to Understand Likelihood of High Moderation, Slow Assembly Criticality

Given enough time, groundwater corrosion or geological processes will breach the waste package and allow groundwater to enter. Water can leach neutron absorbers and uranium from the waste packages. Differential migration of highly enriched uranium and neutron absorber through the repository could lead to either separation of neutron absorber from highly enriched uranium fuel remaining at the container location or deposition and concentration of highly enriched fuel elsewhere. Either circumstance creates the potential for a criticality within the repository.

As argued in Sections 10.2 and 10.4 in which possible types of critical events were presented, an actual repository criticality would more likely be portrayed as a slow rise toward $k_{\text{eff}} \sim 1$, and then low-power production of neutrons for a finite period of time, self-shutdown for a period, and then perhaps a repeat through a number of cycles. In the bounding calculations, a conservative analysis was used to estimate a bounding limit for the fission energy released over 10,000 yr due to criticality excursions within emplaced waste containers. That model treated the energy release process as steady state without taking into account the thermodynamics and the thermal-hydraulics of the repository. Although the steady-state calculations above bound the maximum energy release over 10,000 yr, it may not be credible that a natural reactor could produce energy continuously over such a long time period. Maintaining a critical condition depends upon availability of water, ability to dissipate heat, etc. Changes to any of these processes could stop the reaction until conditions conducive to a new reaction were reestablished. Evaluating the energy release from this dynamic situation became the goal of the third criticality model.

A complete evaluation of the processes leading to a critical condition should include dynamic changes in the controlling parameters: fuel amount, fuel shape, water mass, and temperature. Although this type of model was beyond the scope of the 1994 PA, some calculations were manually coupled with the thermal and hydrologic flow

code in the unsaturated zone. These calculations explored how much time was needed after a critical event for optimal conditions to reoccur, i.e., for temperatures to drop and sufficient water to collect again around a container.

The computational and decisional steps needed for this modeling are shown in Figure 10-5 and described below. Discussion of the computational models are described in the following sections, which explore various phenomena leading up to highly moderated, slow assembly criticalities. Section 10.6 explores the interaction of various phenomena acting during a highly moderated, slow assembly criticality.

10.5.1 Steps for Determining Dynamics of a Critical Event in a Repository

The following steps occurred in examining various phenomena leading up to and during a highly moderated, slow assembly criticality (Figure 10-5). The section following provides more details on the methods used and the results of these steps.

Step 1: Calculate Failure Times of Containers. Calculations for the corrosion chemistry are performed to identify the amount of time necessary for corrosion breakthrough of the repository container. If corrosion breakthrough of the container does not occur within the regulatory period (10,000 yr after disposal), then further calculations are not necessary.

Step 2: Evaluate Boron (Neutron Absorber) and Uranium Solubility in Tuff Groundwater. Detailed calculations are performed to determine (1) the solubility of fissile material (uranium) in the groundwater, and (2) the solubility of neutron absorbing material (boron) in the groundwater.

Step 3: Calculate Removal of Uranium and Boron from Containers. The calculations in this step are by far the most important calculations in this series. Here, solubilities and corrosion models are used with distributions for the groundwater flux going through the fuel region. Although the models may be the same as the corrosion models used in Step 1, here they model the corrosion of (1) inner basket regions of handling containers that contain neutron absorbers, (2) fuel cladding or confinement material, and (3) the fuel itself. At the end of this step, one can determine whether the fissile material that has washed away is more significant than the neutron absorbers.

Step 4a: Identify Mineral Precipitate. This computational step is used only for the case in which fissile material is transported away from the repository container in greater quantities than neutron absorbers (see Step 3). From geochemical calculations, various uranium mineral precipitates are identified. The most likely of these precipitates are identified; atom number density calculations are made for this mineral precipitated within the tuff.

Step 4b: Calculate Time to Remove Boron for Criticality in Container. In Step 4b, the time to remove various quantities of boron is calculated. This step is used only for the case in which neutron absorbers are transported away from the repository container in greater quantities than fissile material (see Step 3).

Step 5a: Calculate Critical Masses in Pores of Tuff. Using the information from Step 4, Monte Carlo neutron transport calculations are run to identify the mass of fissile material necessary to generate a critical assembly.

Step 5b: Calculate Required Mass of Boron to Prevent a Criticality. As in Step 5a, calculations are done, or previous calculations on designing the packing within containers are used, to identify the mass removal of neutron absorber necessary to permit a critical assembly.

Step 6: Identify Most Likely Fuel Type to go Critical. In Step 4, the amount of material (fissile or neutron absorber) is identified that must be transported from the waste container in order for a critical situation to occur. Using the leaching rate distributions (Step 3), it is possible to determine if a critical assembly can occur within the regulatory period. If so, then the most likely fuel type to yield a critical assembly can be identified. The geometry associated with the most likely case is then used for Step 7.

10.5 Process Modeling to Understand Likelihood of High Moderation, Slow Assembly Criticality

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Figure 10-5. Computational steps for determining dynamics of a critical event in a geologic repository.

Step 7: Evaluate Disruption of Fluid Flow. Ideally the fluid flow, the nuclear kinetics, and the evaluation of the multiplication factor (k_{eff}) would be coupled together in a single code to yield the proper nuclear dynamics response. Instead, a manually coupled series of calculations is performed.

In Step 7, a selected series of fluid flow calculations is performed for the most likely fuel type identified in Step 5. The calculations are designed to be compared to results from a nuclear kinetic model. For these calculations, the expected power history would likely be similar to Figure 10-4.

The fluid flow calculations are performed for various total integrated energies. For each integrated energy, several combinations of pulse shapes were used. The output from the thermal hydraulic analysis yields temperature and saturation information as a function of time. These values are used to calculate the effective criticality constant (k_{eff}) as a function of time.

Step 8: Evaluate Likely Dynamics for Natural Reactor. The time history of k_{eff} from Step 7 is used to solve the nuclear kinetics equations to yield a calculated power time history. This computed power history is then compared to the "guessed" power history. A series of iterations on the "guessed" power history is made until matched with the "computed" power history.

The overall results of the calculations are used to identify the maximum energy release expected for a criticality event, and the amount of time necessary for the repository to thermally respond (including groundwater saturation effects) and be capable of attaining a critical assembly again, i.e., return saturation to conditions similar to that prior to the criticality event. From these parameters, the total amount of energy released from nuclear fission is estimated for the regulatory period (10,000 yr). This value, based on dynamic repository response, will be less conservative than the 10,000-yr energy release value determined by steady-state analysis (see Section 10.4.2).

Step 9: Evaluate Effects of Heat and Inventory. As with the steady-state calculations, the final step is to evaluate the effects of the heat and additional radionuclide inventory on the tuff disposal system.

10.5.2 Container Failure (Step 1)

As outlined in Figure 10-5 and Section 10.5.1, the first step performed as part of the investigation of the nuclear dynamics of the repository was the identification of the failure times of the canisters. Obviously, if the canisters do not experience corrosion breakthrough within the 10,000-yr period, then a nuclear criticality due to corrosion processes would not be possible. The calculations for identifying the corrosion failure times were performed with the complete structure of PA codes. The analysis was performed with a detailed model that included processes such as groundwater flow, corrosion chemistry, and solubility chemistry (see Chapter 15). Input parameters were Monte Carlo sampled to yield results that indicated that corrosion breakthrough of the repository canisters is possible within the 10,000-yr period. The Monte Carlo sampling was performed for nine different waste packages, four different container groups, and 38 individual grid blocks. Because the failure time is strongly dependent on several parameters, it is not possible to generate a single distribution function for the waste container failures. Additional discussion on this topic is provided in Chapter 15. The primary fact of interest in regard to criticality is that corrosion breakthrough was identified to occur within the 10,000-yr period for a portion of the containers.

10.5.3 Boron and/or Uranium Solubility (Step 2)

A crucial analysis effort was the identification of the release rate of the neutron absorbers (boron) and solubility of fissile materials within the groundwater. These parameters, together with groundwater flux rates, can then be used to determine the cumulative leaching of neutron absorber and the fissile material. The solubilities for these materials in silica-rich groundwater has not been measured in repository-like conditions and must be calculated. These calculations were performed with the code, EQ3/6. The obtained solubilities are shown in Table 10-11.

Table 10-11. Median Solubilities for Plutonium, Uranium and Boron (see Chapter 11)

Element	Non-Silicic Solubility* (log) (M)	Silicic Solubility (log) (M)
Plutonium	-7.000	-11.75
Uranium	-4.500	-5.925
Boron	1	1

* Constant temperature of 298 K

Boron as Chromium-Boride. Preliminary investigation of the metallurgy of borated stainless steel (used in the support structure) indicated that during the formation process at high temperatures, the boron atoms assume grain boundary locations that lead to the generation of chromium-borides (i.e., the boron atoms combine with chromium atoms in the stainless steel in the same manner that carbon atoms have been observed to combine with chromium atoms to form chromium-carbides). When the container support structure corrodes, the boron in the form of chromium borides, is released very slowly to the groundwater (additional discussion can be found in Chapter 11).

Leaching Process. When the oxygen is assumed to be readily available, the leaching of fissile and boron material was perceived to occur as follows:

- Silica-saturated groundwater comes into contact with the disposal canisters.
- Canister corrosion proceeds.
- After canister corrosion breakthrough, silica-saturated groundwater enters the corroded canister. As it enters the canister, the change in environment results in silicates being precipitated from the groundwater. The groundwater is no longer as highly saturated in silica and is now more amenable for leaching some of the contents of the corroded canister.
- Leaching of the fissile material (after cladding corrosion) and boron material can now proceed. Because the boron available for leaching is in the form of chromium-boride (which has a slow alteration rate), the amount of boron leached during the regulatory period of 10,000 yr as computed is relatively insignificant. Thus, fissile material is identified as being the leached species of concern. Even though fissile material is being transported in much greater quantities than the boron material, the total amount of fissile material leached from the disposal canisters is not large.
- Once fissile material is in solution, it can be transported away from the corroded canisters. When this solution enters a far field location (which may be as close as several meters away from the canisters) the now fissile-enriched groundwater enters an environment in which the groundwater is saturated in silica. At this point fissile material will be precipitated out within fractures and/or pores of the host rock (tuff material in this study).

Currently available transport models are not capable of identifying the concentration, shape, and/or location of fissile precipitation zones. (A key complication in the models is that there is not a lot of available groundwater for the leaching process and knowledge of the shape of the associated probability density function is limited.) Should enough fissile material be accumulated to achieve a critical mass, then a "nuclear dynamics" situation would occur.

10.5.4 Removal of Uranium and Boron from Containers (Step 3)

To achieve a self-sustaining nuclear chain reaction, a significant concentration of fissile material (e.g., ^{235}U , ^{239}Pu) in an appropriate geometry is required. As already mentioned, it would not be possible to achieve a situation conducive to criticality except for effects from water corrosion and chemistry. The containers used for the repository disposal are designed to maintain a subcritical assembly with an appropriate safety margin even when flooded with water. However, unlike conditions for above-ground storage or transportation, the repository may include inundated or partially saturated conditions that are conducive to the corrosion of the containers. Once corrosion breakthrough

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has occurred, the groundwater chemistry and transport might lead to the development of a critical assembly of fissile material. Two possibilities exist for forming a critical assembly: (1) the groundwater chemistry may be such that the neutron absorber materials in the canister would leach out (go into solution and become transported) in much greater rates than the fissile material or (2) vice versa. The near-field critical assembly (which could be only centimeters away from the waste containers) is possible only if the right combination of transport mechanisms and Eh/pH conditions exist to allow fissile material to be concentrated and precipitated out in significant quantities and in an appropriate geometry. For a near-field precipitation zone that is within the pore space of a host rock formation, the mass of fissile material would have to be very large because of the hindrance of the host rock (i.e., the host rock would greatly absorb neutrons without contributing to fissions), as calculated in Section 10.5.5.

At the end of Step 3, the leach rates of the fissile material and the neutron absorber are compared. This step is designed to identify if enough fissile material to generate a critical assembly outside the container occurs prior to the removal of enough neutron absorber to cause a critical assembly inside the container. Although borates are known to be very soluble, the alteration rates of metal borides are unknown.

Flow Rate Around the Waste Container. ^{††} Using the rain infiltration model currently implemented in the Complex PA calculations, cumulative probability and probability density functions for the volumetric flow rates around waste parcels in the waste disposal group for vertical orientation were computed at 10,000 years (year 12,030). The cumulative probability and probability density functions of the volumetric flow rates are shown in Figure 10-6. As seen in the figure, the volumetric flow rates around the waste parcels have a mean and median value of $7.21 \times 10^{-5} \text{ m}^3/\text{yr}$ and $5.52 \times 10^{-5} \text{ m}^3/\text{yr}$, respectively. Three of the BRAGFLO_T rain infiltration model parameters, $I_{\min}$, $I_{\max}$, and τ of Equation 10-3 (see also Figure 5-7, Chapter 5),

$$I = I_{\min} + \left(\frac{I_{\max} - I_{\min}}{2} \right) \cdot \left[1 - \cos \left(\frac{2\pi t}{\tau} \right) \right] \quad (10-3)$$

were sampled (using LHS). The rain infiltration rate, I , represents the maximum rate that water from the surface can reach the repository at any time, t . The BRAGFLO_T calculations incorporated a "focus-point" into Equation 10-3 which results in the maximum flow into the repository. Combining Equation 10-3 and waste parcel collection areas, a volumetric flow rate cumulative probability function and probability density function were constructed using a data distribution as,

$$\dot{q}_{awp} = I \cdot A_c \quad (10-4)$$

where

- I = rain infiltration rate in the vertical direction [m/yr],
- A_c = waste parcel collection area [m²],
- $\dot{q}_{awp}$ = volumetric flow rate around waste parcels [m³/yr].

Estimated Removal. Results for the cumulative fissile mass removed are presented in Figure 10-7 and Table 10-12. The fraction of boron removed in the same simulations was several orders of magnitude below uranium; hence, it appears uranium would be dissolved and transported before boron. It is important to note here that the boron mentioned is in the chemical form of chromium boride.

The results are interesting in that they indicate that the median value is on the order of 10 kg of ²³⁵U Fissile Gram Equivalent (FGE) (see Appendix H) that can be transported over 10,000 yr for all the waste parcels combined, assuming the composite porosity model and concentrating infiltration from climate change (Equation 10-3).^{***} This median value of mass available for precipitation of between 10 and 100 kg for all highly enriched containers (discussed in Section 10.6.1) was used in subsequent calculations.

^{††} The results obtained in this study do not indicate that it is necessary to have 10,000-yr design life container in order to prevent a criticality induced violation of regulatory limits.

^{***} A separate study increasing the volumetric flow rates beyond those here only increased results by 1 order of magnitude for the mass released.

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Figure 10-6. Estimated distribution (cdf and pdf) for global flow rate from sampled parameters of climate change and concentration of infiltration from resulting precipitation.

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Figure 10-7. Cumulative ^{235}U mass leaching from waste parcels. Volume flow rates vary according to Latin Hypercube Sampling infiltration.

Table 10-12. Minimum and Maximum Mass Removed from Containers over 10,000 Yr

Isotope	Minimum Mass Leached from All Waste Parcels* (kg)	Maximum Mass Leached from All Waste Parcels* (kg)
^{233}U	2.67×10^{-5}	0.419
^{234}U	2.07×10^{-4}	3.36
^{235}U	3.01×10^{-2}	7.28×10^3
^{236}U	3.11×10^{-3}	4.28×10^1
Eq ^{235}U (FGE)**	3.22×10^{-2}	7.28×10^3
Boron	n/a	n/a

* After 10,000 yr.
**Fissile gram equivalent (see Appendix H); see also Figure 10-7.

10.5.5 Evaluate Critical Masses of Precipitation or Removal (Step 4a)

Probable Uranium Mineral Phases. The main solubility limited phase in the oxic system with a pH range of 7 to 9 and silica saturation of 1×10^{-3} M is soddyite $[(\text{UO}_2)_2(\text{SiO}_4) \cdot 2\text{H}_2\text{O}]$, a uranyl silicate. Schoepite $(\text{UO}_3 \cdot 2\text{H}_2\text{O})$ an oxide hydrate, and soddyite act as limiting phases if aqueous silica is depleted from the solution. Soddyite and $\text{UO}_2(\text{OH})_2(\text{beta})$ alternate as the dominant limiting phase in a system if silica is depleted from the aqueous solution. The solubility of the uranium varies as a function of the aqueous silica in solution, but as long as sufficient $\text{SiO}_2(\text{aq})$ exists to support the precipitation of U-silicates the uranium concentration is maintained at less than 1×10^{-8} M.

Table 10-13 lists potential uranyl phase precipitates used in criticality calculations. A ranking was done to show the potential for each phase.

Topopah Spring Tuff Mineralogy. To accurately establish conditions for criticality, the composition of the repository rock was required. The repository rock was modeled after the Topopah Spring Tuff from the Yucca Mountain Project, which is a densely welded, devitrified silicic tuff. The dominant minerals in the Topopah Spring Tuff are silica polymorphs (tridymite, opal-CT, cristobalite, and quartz), clinoptilolite, sanidine, mordenite, analcime, and clays. The three major phases, quartz, sanidine (alkali feldspar), and cristobalite, make up 98% of the host rock (Delany, 1985). Table 10-14 summarizes the major phases of the Topopah Spring Tuff. (Further description is found in Section 11.4.)

The analytic compositions and bulk volume estimates of the major phases used were from an average of quantitative estimates made from petrographic and x-ray diffraction observation (Delany, 1985). The grain density of Topopah Spring Tuff was computed to be 2485 kg/m^3 . Using a median porosity (ϕ) of 13.9% yields a bulk density of 2140 kg/m^3 . The compositions of alkali feldspar, plagioclase, and biotite are represented as solid solution compositions in the tuffaceous rock (see Tables 10-15 and 10-16 below). Mg-beidellite was used because it takes into account the major cation concentration in the chemical formula.

Table 10-13. Uranium Potential Phases

Mineral	Density (kg/m ³)	Composition	Ranking
Soddyite	5090	(UO ₂) ₂ (SiO ₄)·2H ₂ O	1*
Schoepite	4870	UO ₃ ·2H ₂ O	2*
Haiweeite	3350	Ca(UO ₂) ₂ (Si ₂ O ₅) ₃ ·5H ₂ O	3*
Schoepite-dhy	6550	UO ₃ ·H ₂ O	4
Uranophane	3410	Ca(UO ₂) ₂ (SiO ₃) ₂ (OH) ₂	5
Rutherfordine	5720	UO ₂ CO ₃	6
Uraninite	10,970	UO ₂	7
Boltwoodite	4370	KH ₃ OUO ₂ SiO ₄	9
Coffinite	7160	USiO ₄	8
Weeksite	4020	K ₂ (UO ₂) ₂ Si ₆ O ₁₅ ·4H ₂ O	10

* Designates solid phases most stable for J-13 well water at Eh = 0.7 V and pH range of 7 to 9. Temperatures ranged from 25°C to 100°C.

Table 10-14. Composition of the Topopah Spring Tuff*

Phase	Composition**	Density (kg/m ³)	Volume (%)
Cristobalite	SiO ₂	2330	44
Alkali Feldspar	Or _{0.58} Ab _{0.41} An _{0.01}	2580	39
Quartz	SiO ₂	2650	14.9
Plagioclase	Or _{0.07} Ab _{0.76} An _{0.17}	2630	1
Mg-Beidellite	Mg _{1.65} Al _{2.33} Si _{3.67} O ₁₀ (OH) ₂	2950	1
Biotite	Ph _{0.43} Ann _{0.57}	3090	0.1
Total			100.0

* Data from Delany, 1985.

** Subscripts denote volume fractions; see Table 10-15 for Feldspar composition.

Table 10-15. Feldspar Composition*

Mineral	Composition	Density (kg/m ³)
Orthoclase (Or)	KAlSi ₃ O ₈	2550
Albite (Ab)	NaAlSi ₃ O ₈	2620
Anorthite (An)	CaAl ₂ Si ₂ O ₈	2710
* Data from Delany, 1985.		

Table 10-16. Biotite Composition*

Mineral	Composition	Density (kg/m ³)
Phlogopite (Ph)	KMg ₃ AlSi ₃ O ₁₀ (OH) ₂	2790
Annite (Ann)	KFe ₃ AlSi ₃ O ₁₀ (OH) ₂	3320
* Data from Delaney, 1985.		

The compositions of the feldspar minerals are given in Table 10-15. The chemical compositions are expressed in terms of molecular percentages of orthoclase, albite, and anorthite.

The composition of biotite is given in Table 10-16. The chemical composition is expressed in terms of molecular percentage of phlogopite and annite.

Table 10-17 lists the constants used to calculate the density and molecular weight of the rock. These values are taken from the DATAO.COM file of EQ3/6 thermodynamic data base.

Table 10-17. Constants Used to Construct the Rock Composition*

Mineral	Density (kg/m ³)	Molecular Weight
Cristobolite	2330	60.084
Alkali Feldspar	2580	271.771
Quartz	2650	60.084
Plagioclase	2630	266.151
Mg-Beidellite	2950	363.96
Biotite	3090	471.197
* Data from Wolery, 1992a.		

Isotopic Breakdown of Fuels. Also needed was the isotopic breakdown of the uranium fuels. For this computational effort, three fuel types were considered: highly enriched uranium (HEU), uranium in graphite fuels, and low enriched uranium (LEU) fuel. The isotope breakdown of these fuels is summarized in Table 10-18.

Table 10-18. Isotopic Breakdown of Fuel Types^a

Fuel Type	Isotope	Abundance (wt fraction)
Highly enriched uranium ^b	²³³ U	8.10472×10^{-8}
	²³⁴ U	1.42952×10^{-4}
	²³⁵ U	0.796461848
	²³⁶ U	0.109335371
	²³⁸ U	0.094059746
Graphite ^c	²³³ U	0.200354712
	²³⁴ U	0.039614064
	²³⁵ U	0.533431563
	²³⁶ U	0.147565982
	²³⁸ U	0.078988601
Low enriched uranium ^d	²³³ U	6.04815×10^{-9}
	²³⁴ U	2.18363×10^{-4}
	²³⁵ U	8.321152×10^{-3}
	²³⁶ U	4.145338×10^{-3}
	²³⁸ U	0.98731514

^a Weight fractions obtained from radionuclide data from the 1993 PA database (Rechard, Ed., 1993).

^b Highly enriched uranium fuel from the Advanced Test Reactor (ATR).

^c Graphite fuel from the Fort St. Vrain reactor.

^d Low enriched uranium fuel corresponding to a typical pressurized water reactor (PWR).

10.6 Reactor Dynamics

Section 10.6 continues steps outlined in Section 10.5 for the analysis of a natural reactor. This section explores the various phenomena acting *during* a highly moderated, slow assembly criticality; specifically, the neutron transport, reactor dynamics calculations, and fluid flow calculations that were performed.

The critical event examined in these calculations is for a near-field situation of fissile material in a highly saturated environment. It is assumed that absorbers have leached from the container or that the absorbers remain but the uranium has been transported. The dynamics of a repository are different from the dynamics in a reactor, in which conditions and materials are precisely defined. Geochemistry processes are the most significant and least predictable of the processes that need to be modeled in order to identify the shape and chemical composition of a critical assembly of fissile material within the host rock. Thus these calculations assumed the shape of the uranium is a sphere (worst-case geometry).

The calculations were performed to determine (1) the temperature rise of the near-field components, (2) the thermal-hydraulic response of the geologic system, i.e., the movement and vaporization of water, (3) the recovery time of the geologic system, i.e., the duration of time needed for temperatures to drop and for water to flow back into the near-field system in sufficient quantities such that a criticality can occur again, and (4) the energy release per nuclear excursion. It does not appear that a cyclic period with excursions typical of an accident would occur; it would require

a much smaller number of fissions in each critical excursion in unsaturated tuff. However, the calculations indicated that any significant changes in the groundwater saturation of the host rock would result in large system reactivity changes. Thus any thermal heating large enough to make a groundwater saturation as low as 1% by volume would rapidly shut down the nuclear heating. The self-shutdown (negative feedback) mechanisms are so large that it was not possible to create a criticality excursion that would yield a large fission release. Instead, various large fission releases (between 10^{18} and 10^{21} fissions) were forced to estimate upper bounds for the thermal-hydraulics.

These limited calculations yielded information on the temperature rise, the groundwater saturation, and the recovery time of the system (i.e., the duration of time needed for the system to recreate the initial conditions). For example, these calculations explored how much time was needed after a critical event for optimal conditions to reoccur, i.e., for temperatures to drop and sufficient water to collect again around a container. A critical event was assumed at 10^{19} fissions, which is similar to the release observed in documented criticality accidents, yielding a duration of critical excursion of 4 days and a cycling time period of about 70 days, which results in a maximum energy release over 10,000 yr of about 10^{24} fissions.

10.6.1 Required Mass of Precipitate Outside Container (Step 5b)

Many Monte Carlo calculations for k_{eff} were performed with the computer code MCNP (Briesmeister, 1986, 1988). These calculations primarily focused on identifying various combinations of geometries, uranium precipitate concentrations, and water saturation that could yield a critical assembly. For the calculations, the host rock material was Topopah Spring Tuff with a median bulk porosity of 13.9%. Only the uranium mineral precipitates that were most expected (soddyite and schoepite) were analyzed. All calculations were performed for highly enriched uranium fuel only. The decision was made because (1) the leach rate analyses indicated that between 10 and 100 kg of ^{235}U FGE would be leached over 10,000 yr (thus indicating that the low enriched uranium would not be leached in sufficient quantities to reach a critical mass accumulation) and (2) the graphite fuel is comprised of ceramic-coated fuel particles emplaced within graphite and it is difficult to alter the ceramic coating to dissolve uranium material out of these particles.

Mathematical Formulation for Evaluating Critical Masses. This section discusses the concepts behind the results described above to evaluate the multiplication factor (k_{eff}) of various diameter spheres of uranium mineral deposits in pores of tuff (based on the mineralogy of the tuff described in Section 10.5.5) at several levels of saturation. The two general approaches to criticality calculations are diffusion theory and transport theory (i.e., use of the Boltzmann transport equation). Diffusion theory is used extensively in reactor situations, but has limitations with respect to criticality safety purposes. For diffusion theory, the calculations for critical reactor sizes correspond to a search for eigenvalues that satisfy the differential equation that describe the diffusion process. The first value (fundamental eigenvalue) describes the flux profile in a minimum size critical reactor. This is shown in Equations 10-5 through 10-9 below (note that Equation 10-7 is the eigenvalue or Helmholtz equation):

Diffusion Equation (one-speed formulation):

$$\left\{ \begin{array}{l} \text{time rate} \\ \text{of change} \\ \text{of neutrons} \end{array} \right\} = \left\{ \begin{array}{l} \text{source} \\ \text{term} \end{array} \right\} - \left\{ \begin{array}{l} \text{neutron} \\ \text{leakage} \end{array} \right\} - \left\{ \begin{array}{l} \text{neutron} \\ \text{absorption} \end{array} \right\} + \left\{ \begin{array}{l} \text{extraneous} \\ \text{neutron} \\ \text{source} \end{array} \right\} \quad (10-5)$$

$$\frac{\partial n}{\partial t} = k_{\infty} \Sigma_a \phi - (-D \nabla^2 \phi) - \Sigma_a \phi + S, \quad (10-6)$$

where,

- k_{∞} = new thermal neutrons that appear for each neutron absorbed (for an infinite medium)
- D = diffusion constant
- ϕ = neutron flux

or (for steady-state conditions):

$$\nabla^2 \phi + B^2 \phi = 0 \quad (10-7)$$

where,

$$B^2 = \frac{k_{\infty} - 1}{L^2} \quad (10-8)$$

$$L = \sqrt{D/\Sigma_a} \quad (10-9)$$

Transport theory, on the other hand, is usually applied through discrete ordinates or Monte Carlo formulations. The time-dependent transport theory (Boltzmann Equation) is given by:

$$\frac{\partial n}{\partial t} + v \hat{\Omega} \cdot \nabla n + v \Sigma_t n(r, E, \hat{\Omega}, t) = \int_{4\pi} d\hat{\Omega}' \int_0^{\infty} dE' v' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) n(r, E' \hat{\Omega}', t) + s(r, E, \hat{\Omega}, t) \quad (10-10)$$

where,

r	=	neutron position vector
E	=	neutron energy
$\hat{\Omega}$	=	solid angle
t	=	time
n	=	neutron population
v	=	number of neutrons per fission
Σ	=	macroscopic cross-section = atom density $\times$ microscopic cross-section

Discrete ordinates codes solve the Boltzmann equation by dividing the neutron directional dependence into groups, neutron energy values into limited number of energy groups and using a grid of spatial mesh points (usually regular rectangular or cylindrical mesh arrangements). These limitations lead to applications for only simple geometries. The difficulty in obtaining numerical solutions to the Boltzmann equation in complex geometries has led to the widespread use of Monte Carlo methods for the simulation of particle interactions.

For the 1994 PA, criticality calculations (eigenvalue calculations) performed at Sandia are done with the Monte Carlo computer code: MCNP (A General Monte Carlo Code for Neutron and Photon Transport, Version 4a). MCNP is a general-purpose, continuous-energy, generalized-geometry, time-dependent, coupled neutron/photon Monte Carlo transport code (Group MCNP, 1981; Briesmeister, 1986, 1988). MCNP solves neutral particle transport problems and can be used in any of three modes: neutron transport only, photon transport only, or combined neutron/photon transport, where the photons are produced by neutron interactions. The neutron energy range is from 1.0×10^{-11} MeV to 20 MeV, and the photon energy regime is from 1 keV to 100 MeV. The capability to calculate k_{eff} eigenvalues for fissile systems is also a standard feature.

The code uses the Monte Carlo method both in particle track simulation and in particle interaction simulation. It is a high fidelity code and is currently the leading state-of-the-art in neutron and photon transport calculations because it uses pointwise cross sections in addition to the multigroup cross sections that are used by other Monte Carlo neutronic codes (i.e., KENO-V and MORSE [Straker et al., 1970]). MCNP has been used and benchmarked by radiation scientists for many years and the architecture and physics modules in MCNP are considered to be of good quality.

The geometry component of MCNP allows explicit modeling of complex 3-dimensional configurations through combinatorial geometry input. The unique ability of the Monte Carlo method to calculate neutron multiplication for highly irregular geometries has made it particularly useful for nuclear criticality safety. Incorrect geometry is identified by the code during execution or can be determined prior to execution from a graphics display code.

For nuclear criticality calculations, the Monte Carlo procedure is applied by developing a model that is capable of "tracking" individual (fictitious) neutrons through a material medium containing fissile and other species. A complete description of neutron travel paths accounts for types of and distances between interactions; energies and directions of travel; production from fission or other reactions; and loss by capture or leakage. Each event may be described or otherwise characterized by such familiar parameters as reaction cross sections, mean free paths, scattering distributions, and energy spectra.

Continuous-energy (or pointwise) neutron cross-section data for use in Monte Carlo calculations are available to MCNP from several libraries. The physics of the interactions for each element or radionuclide is contained in these neutron cross-section sets. The cross-section data depend on incident neutron energy and are tabulated at a number of energy points sufficiently dense that linear-linear interpolation at intermediate energies represents the desired quantity to within certain specified tolerances. Each cross-section set is generated from an evaluated data set and is then stored with a unique identifier (the ZAID number) on one of the several libraries. The evaluated data come from many sources: ENDF/B-III, -IV, -V (Garber, 1975), ENDL-73, -75, -76, -79, -85 (Howerton et al., 1975), AWRE (Parker, 1963), as well as special Los Alamos evaluations. In general, cross sections (whether continuous or discrete) based on ENDF/B-V evaluations are believed to be the best available to MCNP users at this time. Therefore the default cross sections for MCNP are based upon the ENDF/B-V evaluations, although in some cases the ENDF/B-V sets are supplemented by more recent evaluations from T-2 (the Applied Nuclear Science Group at Los Alamos National Laboratory). Because the Monte Carlo method is statistical in nature, the results are characterized by a standard deviation proportional to the square root of the number of events (similar to the typical $n \pm \sqrt{n}$ reported for a radiation counting experiment, i.e., Poisson statistics). The relationship between precision and computational costs depends on the number of histories (number of particles monitored from birth to death) where a gain of 2 in precision costs a factor of 4 in computer time.

10.6.2 Identify Most Likely Candidate for a Criticality (Step 6)

As described above, the maximum amount of ^{235}U FGE from all the waste parcels is on the order of 10 to 100 kg. The critical results shown in Table 10-19 indicate that there are various fissile-water-void combinations that can result in a critical assembly under the 7 kg limit (for highly enriched uranium spent fuel only). Also, the results for soddyite do not differ significantly from those for schoepite. Therefore, a choice for a criticality was assumed to be an 80-cm-diameter spherical geometry of Topopah Spring Tuff with soddyite precipitation (from highly enriched fuel), comprising 0.4% by volume of the tuff/unit volume (see Table 10-19).

Included in Table 10-19 were a set of calculations for this geometry (corresponding to about 3.09 kg of ^{235}U FGE) for various conditions of saturation. The calculated k_{eff} values from this simple model indicated a strong dependence on saturation. This dependence means that groundwater saturation losses would be a strong self-shutdown mechanism should a critical assembly form (which would require large amounts of integrated water flow along with favorable precipitation conditions) and generate any significant amounts of heat.

10.6.3 Perform Thermal Hydraulics Calculations (Step 7)

Results. Of all steps identified (Figure 10-5), Step 7 proved to be the most difficult to perform. The fundamental problem in performing the required nuclear dynamic and thermal-hydraulic calculations is the sensitivity of the nuclear assembly to small changes in reactivity near $k_{\text{eff}} = \text{unity}$. Very small positive reactivity insertions (i.e., k_{eff} is slightly above unity) results in power levels that begin to cause the temperature of the immediate region to rise; however, any significant temperature rises result in changes in the water saturation. As suggested in the previous section, even minor changes in saturation have dramatic changes in reactivity. To illustrate this, a base case was chosen for study that corresponds to Topopah Spring Tuff (13.9%) with 0.4% of soddyite mineral within the pores of the tuff. Extracting selected data from Table 10-19 and redisplaying it to include saturation yielded Table 10-20 and Figure 10-8. From the figure it can be seen that a reduction in saturation from $S_w = 85\%$ to $S_w = 84\%$ has a major criticality impact, corresponding to a decrease of k_{eff} from near unity to 0.998. This decrease computes to a reactivity change of -0.31% ("31¢"). This easily shuts down the power generation of the nuclear assembly.

Table 10-19. Required Sphere Diameter and Fissile Gram Equivalents of Soddyite and Schoepite Uranium Precipitates to go Critical in Topopah Spring Tuff with a Porosity of 13.9% *

Materials in Tuff ($\phi_{\text{total}} = 13.9 \text{ vol. \%}$)			Required Precipitation Sphere Diameter (cm)	²³⁵ U fissile gram equivalents in sphere (kg)	Hydrogen/ ²³⁵ U Ratio	Calculated Multiplication Factor ($k_{\text{eff}} \pm s$)**
Fissile (Vol. %)	Water (Vol. %)	Void (Vol. %)				
Soddyite						
0.4	13.5	0.0	20.0	0.048	311.45	0.08939 ± 0.00088
0.4	13.5	0.0	40.0	0.39	311.45	0.52493 ± 0.00224
0.4	13.5	0.0	60.0	1.30	311.45	0.85428 ± 0.00243
0.4	13.5	0.0	80.0	3.09	311.45	1.02553 ± 0.00257
0.4	12.5	1.0	80.0	3.09	288.85	1.01863 ± 0.00240
0.4	12.15	1.35	80.0	3.09	280.86	1.00981 ± 0.00118***
0.4	11.88	1.62	80.0	3.09	274.75	1.00598 ± 0.00117***
0.4	11.745	1.755	80.0	3.09	271.69	1.00684 ± 0.00120***
0.4	11.61	1.89	80.0	3.09	268.63	1.00355 ± 0.00125***
0.4	11.475	2.025	80.0	3.09	265.57	1.00146 ± 0.00124***
0.4	11.34	2.16	80.0	3.09	262.51	0.99752 ± 0.00125***
0.4	10.80	2.7	80.0	3.09	250.28	0.99106 ± 0.00120***
0.4	11.5	2.0	80.0	3.09	266.14	0.99696 ± 0.00222
0.4	10.5	3.0	80.0	3.09	243.48	0.98621 ± 0.00266
0.4	9.5	4.0	80.0	3.09	220.82	0.96431 ± 0.00258
0.4	8.5	5.0	80.0	3.09	198.17	0.94235 ± 0.00234
0.4	7.5	6.0	80.0	3.09	175.51	0.91840 ± 0.00292
0.4	13.5	0.0	100.0	6.03	311.45	1.21591 ± 0.00227
0.9	13.0	0.0	20.0	0.11	134.78	0.13243 ± 0.00144
0.9	13.0	0.0	40.0	0.87	134.78	0.67976 ± 0.00285
0.9	13.0	0.0	60.0	2.93	134.78	1.04998 ± 0.00292
0.9	13.0	0.0	80.0	6.95	134.78	1.24294 ± 0.00277
0.9	13.0	0.0	100.0	13.6	134.78	1.35770 ± 0.00262
1.9	12.0	0.0	20.0	0.23	60.39	0.16256 ± 0.00147
1.9	12.0	0.0	40.0	1.83	60.39	0.75825 ± 0.00328
1.9	12.0	0.0	60.0	6.19	60.39	1.13795 ± 0.00334
1.9	12.0	0.0	80.0	14.7	60.39	1.33391 ± 0.00304

* The results of this study do not imply that a criticality is inevitable after container failure. The assembly of a critical mass in a geological setting is not very plausible and, if it should occur, would be very difficult to maintain.

** Calculations done with MCNP (Version 4a) using the default value of 10^5 random samples per calculation, except where noted.

*** Calculations done with 4×10^5 random samples.

Table 10-19. Required Sphere Diameter and Fissile Gram Equivalents of Soddyite and Schoepite Uranium Precipitates to go Critical in Topopah Spring Tuff with a Porosity of 13.9% (Continued)*

Materials in Tuff ($\phi_{\text{total}} = 13.9 \text{ vol. \%}$)			Required Precipitation Sphere Diameter (cm)	²³⁵ U fissile gram equivalents in sphere (kg)	Hydrogen/ ²³⁵ U Ratio	Calculated Multiplication Factor ($k_{\text{eff}} \pm s$)**
Fissile (Vol. %)	Water (Vol. %)	Void (Vol. %)				
1.9	12.0	0.0	100.0	28.6	60.39	1.44569 $\pm$ 0.00286
2.9	11.0	0.0	20.0	0.35	37.31	0.17669 $\pm$ 0.00157
2.9	11.0	0.0	40.0	2.80	37.31	0.76056 $\pm$ 0.00342
2.9	11.0	0.0	60.0	9.44	37.31	1.14191 $\pm$ 0.00319
2.9	11.0	0.0	80.0	22.4	37.31	1.33073 $\pm$ 0.00289
2.9	11.0	0.0	100.0	43.7	37.31	1.44313 $\pm$ 0.00172
3.9	10.0	0.0	20.0	0.47	26.06	0.18224 $\pm$ 0.00186
3.9	10.0	0.0	40.0	3.76	26.06	0.75815 $\pm$ 0.00307
3.9	10.0	0.0	60.0	12.7	26.06	1.13048 $\pm$ 0.00313
3.9	10.0	0.0	80.0	30.1	26.06	1.31783 $\pm$ 0.00314
3.9	9.0	1.0	80.0	30.1	23.74	1.28862 $\pm$ 0.00278
3.9	8.0	2.0	80.0	30.1	21.41	1.25678 $\pm$ 0.00286
3.9	7.0	3.0	80.0	30.1	19.09	1.22241 $\pm$ 0.00312
3.9	6.0	4.0	80.0	30.1	16.77	1.17864 $\pm$ 0.00317
3.9	5.0	5.0	80.0	30.1	14.44	1.13831 $\pm$ 0.00326
3.9	4.0	6.0	80.0	30.1	12.12	1.08508 $\pm$ 0.00289
3.9	10.0	0.0	100.0	58.8	26.06	1.42876 $\pm$ 0.00291
4.9	9.0	0.0	20.0	0.59	19.40	0.18628 $\pm$ 0.00172
4.9	9.0	0.0	40.0	4.73	19.40	0.75152 $\pm$ 0.00321
4.9	9.0	0.0	60.0	16.0	19.40	1.11829 $\pm$ 0.00275
4.9	9.0	0.0	80.0	37.8	19.40	1.30039 $\pm$ 0.00301
4.9	9.0	0.0	100.0	73.9	19.40	1.40988 $\pm$ 0.00290
Schoepite						
0.4	13.5	0.0	20.0	0.048	316.20	0.08787 $\pm$ 0.00087
0.4	13.5	0.0	40.0	0.38	316.20	0.52954 $\pm$ 0.00232
0.4	13.5	0.0	60.0	1.29	316.20	0.84462 $\pm$ 0.00287
0.4	13.5	0.0	80.0	3.07	316.20	1.02597 $\pm$ 0.00247
0.4	13.5	0.0	100.0	5.99	316.20	1.12915 $\pm$ 0.00221

* The results of this study do not imply that a criticality is inevitable after container failure. The assembly of a critical mass in a geological setting is not very plausible and, if it should occur, would be very difficult to maintain.

** Calculations done with MCNP (Version 4a) using the default value of 10^5 random samples per calculation, except where noted.

*** Calculations done with 4×10^5 random samples.

Table 10-19. Required Sphere Diameter and Fissile Gram Equivalents of Soddyite and Schoepite Uranium Precipitates to go Critical in Topopah Spring Tuff with a Porosity of 13.9% (Continued)*

Materials in Tuff ($\phi_{\text{total}} = 13.9 \text{ vol. \%}$)			Required Precipitation Sphere Diameter (cm)	²³⁵ U fissile gram equivalents in sphere (kg)	Hydrogen/ ²³⁵ U Ratio	Calculated Multiplication Factor ($k_{\text{eff}} \pm s$)**
Fissile (Vol. %)	Water (Vol. %)	Void (Vol. %)				
0.9	13.0	0.0	20.0	0.11	138.25	0.13504 $\pm$ 0.00154
0.9	13.0	0.0	40.0	0.86	138.25	0.69225 $\pm$ 0.00290
0.9	13.0	0.0	60.0	2.91	138.25	1.05537 $\pm$ 0.00263
0.9	13.0	0.0	80.0	6.90	138.25	1.24823 $\pm$ 0.00300
0.9	13.0	0.0	100.0	14.6	138.25	1.36121 $\pm$ 0.00257
1.9	12.0	0.0	20.0	0.23	63.32	0.17554 $\pm$ 0.00137
1.9	12.0	0.0	40.0	1.82	63.32	0.77071 $\pm$ 0.00341
1.9	12.0	0.0	60.0	6.14	63.32	1.14771 $\pm$ 0.00331
1.9	12.0	0.0	80.0	14.6	63.32	1.33944 $\pm$ 0.00297
1.9	12.0	0.0	100.0	28.5	63.32	1.46071 $\pm$ 0.00319
2.9	11.0	0.0	20.0	0.35	40.07	0.19131 $\pm$ 0.00160
2.9	11.0	0.0	40.0	2.78	40.07	0.79227 $\pm$ 0.00346
2.9	11.0	0.0	60.0	9.38	40.07	1.15935 $\pm$ 0.00359
2.9	11.0	0.0	80.0	22.2	40.07	1.35506 $\pm$ 0.00311
2.9	11.0	0.0	100.0	43.4	40.07	1.46487 $\pm$ 0.00289
3.9	10.0	0.0	20.0	0.47	28.74	0.20355 $\pm$ 0.00162
3.9	10.0	0.0	40.0	3.74	28.74	0.79810 $\pm$ 0.00271
3.9	10.0	0.0	60.0	12.6	28.74	1.15082 $\pm$ 0.00358
3.9	10.0	0.0	80.0	29.9	28.74	1.34704 $\pm$ 0.00311
3.9	10.0	0.0	100.0	58.4	28.74	1.45265 $\pm$ 0.00301
4.9	9.0	0.0	20.0	0.59	22.03	0.21100 $\pm$ 0.00183
4.9	9.0	0.0	40.0	4.69	22.03	0.79763 $\pm$ 0.00299
4.9	9.0	0.0	60.0	15.8	22.03	1.15267 $\pm$ 0.00322
4.9	9.0	0.0	80.0	37.5	22.03	1.33695 $\pm$ 0.00287
4.9	9.0	0.0	100.0	73.3	22.03	1.43626 $\pm$ 0.00273

* The results of this study do not imply that a criticality is inevitable after container failure. The assembly of a critical mass in a geological setting is not very plausible and, if it should occur, would be very difficult to maintain.

** Calculations done with MCNP (Version 4a) using the default value of 10^5 random samples per calculation, except where noted.

*** Calculations done with 4×10^5 random samples.

Table 10-20. Criticality Calculations Performed for Highly Enriched Uranium Spent Fuel in Topopah Spring Tuff, Uranium Mineral Soddyite, Sphere Diameter 80 cm

Materials in Tuff ($\phi_{\text{total}} = 13.9$ vol. %)			Precipitation Saturation (Vol. %)	²³⁵ U fissile gram equivalents in Precipitation (kg)	Hydrogen/ ²³⁵ U Ratio	Calculated Multiplication Factor ($k_{\text{eff}} \pm s$)*
Fissile (Vol. %)	Water (Vol. %)	Void (Vol. %)				
0.4	13.5	0.0	100.0	3.09	311.45	1.02553 $\pm$ 0.00257*
0.4	12.5	1.0	92.6	3.09	288.85	1.01863 $\pm$ 0.00240*
0.4	12.15	1.35	90.0	3.09	280.86	1.00981 $\pm$ 0.00118**
0.4	11.88	1.62	88.0	3.09	274.75	1.00598 $\pm$ 0.00117**
0.4	11.745	1.755	87.0	3.09	271.69	1.00684 $\pm$ 0.00120**
0.4	11.61	1.89	86.0	3.09	268.63	1.00355 $\pm$ 0.00125**
0.4	11.475	2.025	85.0	3.09	265.57	1.00146 $\pm$ 0.00124**
0.4	11.34	2.16	84.0	3.09	262.51	0.99752 $\pm$ 0.00125**
0.4	10.80	2.7	80.0	3.09	250.28	0.99106 $\pm$ 0.00120**
0.4	11.5	2.0	85.2	3.09	266.14	0.99696 $\pm$ 0.00222*
0.4	10.5	3.0	77.8	3.09	243.48	0.98621 $\pm$ 0.00266*
0.4	9.5	4.0	70.4	3.09	220.82	0.96431 $\pm$ 0.00258*
0.4	8.5	5.0	63.0	3.09	198.17	0.94235 $\pm$ 0.00234*
0.4	7.5	6.0	55.6	3.09	175.51	0.91840 $\pm$ 0.00292*

* Calculations obtained with MCNP (Version 4a) using the 100,000 histories, except where noted.

** Calculations obtained with MCNP (Version 4a) using the 400,000 histories.

Greatly compounding the sensitivity of any calculations associated with the self-shutdown mechanisms is the uncertainty (estimated standard deviation) associated with the use of a Monte Carlo computer code to estimate k_{eff} . A selective set of calculations for an extended number of histories was performed to illustrate this (Figure 10-8b). Even with 400,000 histories, sizeable uncertainties exist in comparison to the sensitivity of the effects of changes in saturation. Once the knee in the curve is reached at about 400,000 histories, the extra calculations required to reduce the estimated standard deviation(s) become substantial (i.e., s follow Poisson statistics where a reduction of s by a factor of 2 would require an increase in histories by a factor of 4).

The combination of the ultra-sensitivity of k_{eff} to saturation, combined with the statistical uncertainty of the Monte Carlo results, indicated that Monte Carlo calculations are not an efficient way to couple the thermal hydraulics with nuclear kinetics relationships to yield a nuclear dynamics model (i.e., the complete modeling of the criticality self-shutdown mechanisms). Until a double precision neutron transport code (Pn or Sn discrete ordinates code) or an analytical solution is incorporated, the transient behavior of a precipitation zone critical excursion will have to be estimated through a series of calculations using the thermal-hydraulics code, BRAGFLO_T. The calculations follow the series of steps outlined in Figure 10-5 (Steps 8 and 9).

As previously noted, the dominating physical process is the thermal hydraulics that determines the saturation history of the heat generation zone. The calculations required to determine the time history of the groundwater saturation needed to model the groundwater transport through the host rock by interconnected pores and fractures indicated by changes in fluid density and/or vaporizing of the liquid phase due to heat generation. For these calculations, BRAGFLO_T, a multiphase fluid and energy simulator (see Section 12.1), was used to predict water saturation

TRI-6342-5002-0

(a)

TRI-6342-5010-0

(b)

Figure 10-8. Multiplication factor calculations, (a) multiplication factor versus groundwater saturation, assuming median conditions, and (b) estimated standard deviation as a function of number of samples in Monte Carlo neutron transport code, MCNP.

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changes resulting from a single critical event, of an assumed size and power output. The power output of the event is assumed to be a function of both space and time, which can be defined by the power density function,

$$P(r, t) = P_o \sin(t\pi/T) \cos(r\pi/2r_o) \quad [J/s \cdot m^3] \quad (10-11)$$

where P_o is the power constant [$J/(s \cdot m^3)$], T is the power generation period (s), and r_o = radius of the heat generation zone (m).

The power density function is greatest at the center and reaches a maximum value when the region moves from critical to subcritical conditions (see Figures 10-5 and 10-9).

The size of the events studied varied from 10^{18} to 10^{21} fissions per event. The total energy release, E , for a given event is related to the number of fissions by the conversion factor (from Appendix H), $1J = 3.2 \cdot 10^{10}$ fissions. The power constant, P_o , is found by integrating the power density function over the spherical domain in both space and time, yielding,

$$P_o = \frac{E}{8 T r_o^3 [(2/\pi) - (16/\pi^3)]} \quad [J/(s \cdot m^3)] \quad (10-12)$$

The results of the flow calculations are then tested against a single constraint imposed by the nuclear physics. This constraint is derived from Figure 10-8, where the effect of water saturation on k_{eff} is presented. Fissile matter is considered to be in a critical state when the computed value of k_{eff} is greater than 1. In Figure 10-8, the system will switch from a critical to a subcritical condition when the water saturation changes 0.15. In Figure 10-8, the peak power output occurs during the transition from critical to subcritical conditions. Hence, the peak power output must coincide with a change in average water saturation of 0.15: $\Delta Sw = 0.15$, when $t = T/2$. The period of the power density function, t_s , was chosen such that the results of the flow computations satisfied the last condition. Trial and error produced a solution that satisfied the thermal hydrologic and thermal nuclear physics for a given criticality.

Discretization. A sphere of welded tuff, 1000 m in diameter (see diagram insert in Figure 10-10), within which is a spherical heat-generating region (due to a critical assembly) that is 0.8 m in diameter, is simulated using one-dimensional finite-difference grid blocks. The sphere is discretized in the x direction such that each grid block contains a volume that is roughly 1.5 times larger than the sum of all interior grid-block volumes. Starting with an interior radius of 0.05 m, 70 grid blocks are needed to model a 1000-m-diameter sphere, of which the first 17 grid blocks

TRI-6342-4483-0

Figure 10-9. Power density function, $P(r, t)$, of sphere of fissile material in fluid flow simulation (a) $r \leq r_o$, (b) $t \leq T$.

TRI-6342-5001-0

(a)

TRI-6342-5004-0

(b)

Figure 10-10. Results from calculating possible duration of critical events (a) average saturation for the 1000-m-diameter sphere for 10^{19} , 10^{20} , and 10^{21} fissions, and (b) temperature rises in and outside the sphere for 10^{19} fissions.

contain fissile matter. The spherical geometry is approximated using Cartesian coordinates. Hence element thicknesses (Δz) are computed as a function of the internal and external radius of the grid block to conserve volume. Incorporating symmetry into the problem, only π radians of the sphere are modeled leading to the relationship,

$$\Delta z = \frac{\frac{2}{3} \pi (r_o^3 - r_i^3)}{\Delta x}$$

where r_o is the external radius of an individual gridblock, r_i is the internal radius of an individual grid block, and Δx is equal to $r_o - r_i$.

Initial and Boundary Conditions. The welded tuff is assumed to be nearly water saturated at the beginning of the event. A small amount of gas is placed in the porous media to avoid numerical problems associated with the transition from single-phase liquid to two-phase conditions. The initial conditions were as follows: water pressure, 10^5 Pa; gas pressure, 1.1×10^5 Pa; matrix water saturation, 0.99976; fracture water saturation, 0.05283; and temperature, 26°C .

No flow boundary conditions are imposed on mass flux at both ends of the problem domain. Heat is transported only at the surface of the sphere, using the boundary heat loss option (see Section 12.1.1). At all other boundary locations, no flow boundary conditions are imposed on energy flux.

Results. Calculations indicated that any significant heat generation (corresponding to much less than 10^{18} fissions) will immediately self-shutdown a critical nuclear assembly corresponding to the base case (i.e., 80-cm-diameter assembly of soddyite mineral, 0.4%, within Topopah Spring Tuff at near saturation conditions). This immediate self-shutdown results because the base case geometry is very close to the most optimal (i.e., minimal amount of uranium) geometry and deviations from this geometry (such as loss of water moderator) will shut down the system. If the system was not near the optimal geometry, such as an under-moderated assembly, then it would be less sensitive to changes in the water moderator (e.g., groundwater saturation). This under-moderated assembly would then also be able to experience larger criticality excursions (total number of fissions) before self-shutdown. The under-moderated assembly would require much more uranium mass in order to achieve a critical assembly. However, according to results shown in Figure 10-7, there is not enough leached fuel to accomplish this. It is thus expected that any nuclear assemblies located in the Topopah Spring Tuff would at most experience a large number of extremely small critical excursions. This condition would be much less severe than the situation at Oklo. The fundamental difference between the modeled situation and Oklo is that groundwater was maintained at high pressures at Oklo (lithostatic) and the Oklo natural reactors acted as boiling water reactors. For the tuff disposal system, the tuff's ability to "breathe" allows desaturation to be easily accomplished.

To investigate the thermal hydraulic response of the repository, the power density function was forced to occur over a long period of time. This was done by starting the calculations at a groundwater saturation that is 15% above that needed for a criticality and applying a power density (via Equation 10-31) over a long period of time. The time is selected such that the power peaks when the saturation has dropped 15% to the value just required for a critical situation ($\Delta S_w = -0.15$). By running several power densities, it is possible to identify a power density function that will yield a desired cumulative energy release. After the forced criticality excursion, the assembly requires a duration of time to recover (i.e., to allow the saturation to increase to initial conditions), thus yielding the minimum event cycle time. Results for a selection of calculations are shown in Table 10-21 and Figure 10-10. These calculations are unrealistic in the sense that they require a large drop in saturation (15%) in order to self-shutdown an event. They should give upper limits to integrated fissions.

Reactor Dynamics Mathematical Model. The reactor dynamics modeling incorporates the use of the RNK (Repository Nuclear Kinetics) code, which solves the ordinary differential equations (ODEs) that generate the power history of the repository for a given input criticality history (i.e., k_{eff} vs. time). As identified in Section 10.6.3, a fundamental problem arose that did not allow the RNK code to be coupled to the thermal-hydraulics. The problem was that small changes in groundwater saturation result in large changes in system reactivity. Thus, the calculation of the criticality history from the saturation history must be performed with ultra-precision. As shown in Figure 10-8b, the precision obtained from a Monte Carlo code is limited (even for computations performed with a million histories).

Table 10-21. Summary of Results for Various Thermal-Hydraulic Calculations (a)

Event Fissions (b)	Power Period (c)	Event Cycle Time (d)	Events/ 10,000 yr	Fissions/ 10,000 yr
10^{18} (e)	1 min	0	n/a	n/a
10^{19}	4 days	71 days	51,444	5.1×10^{23}
10^{20}	90 days	143 days	25,542	2.44×10^{24}
10^{21}	1220 days	916 days	3987	3.99×10^{24}

(a) Results obtained with BRAGFLO_T (version 2.00)
 (b) Number of fissions assumed to be released in criticality.
 (c) Calculated power period corresponding to a reduction in groundwater saturation of Δ 15%.
 (d) Duration of time required for $\Delta S_w = +0.14$ (i.e., near initial conditions)
 (e) Not enough energy is released per event to reduce the saturation by 15%.

Because of this difficulty, the RNK code could not be applied at this time. Until a double-precision neutron transport code (Pn or Sn discrete ordinates code) or an analytical solution is incorporated, the transient behavior of a precipitation zone critical excursion can be only estimated (upper bound) through a series of calculations using the thermal-hydraulics code. The following text describes the mathematical model implemented to RNK to calculate the power level of an assembly of fissile material based on the variation of the multiplication factor (k_{eff}) with time.^{†††} This model was to be used to estimate the range of likely cycle periods for a natural reactor within or near a waste container described above. The reactor dynamics physics is modeled by the "classical" point (0-D) kinetics model with feedback. (Note that this is "reactor dynamics" instead of "reactor kinetics" since feedback effects are included in the governing transient equations [Ott and Neuhold, 1971].) The model is non-spatial (i.e., a "lumped" or "point" model) and is commonly used by reactor physicists for engineering level problems. Spatially dependent codes, even one-dimensional codes, are extremely computer intensive and are not needed at the current level of analysis effort. Because this model is a point model, the neutron flux distribution (and hence power density) is taken as a fixed distribution. Using diffusion theory, the flux distribution profile is the "classical" cosine shape (remember that the criticality calculations are eigenvalue calculations that yield the cosine eigenfunction as the first harmonic), thus a first-order estimate of the flux and power distribution is incorporated. The governing equations for the reactor dynamics are derivable from diffusion theory, transport theory, or from a simplified control volume analysis (Keepin, 1965; Henry, 1986; Duderstadt and Hamilton, 1976). The simplest model is the control volume balance in which the time rate of change of neutron population in the reactor is determined from the production rate and loss rate mechanism and is given by Equation 10-10.

$$\frac{dn}{dt} = (1 - \gamma\beta_{eff})k_{eff}\frac{n}{l} + \sum_{i=1}^{N_n} \lambda_i C_i + q_n - \frac{n}{l} \quad (10-13)$$

where

- n = neutron population
- t = time
- γ = delayed neutron energy correction factor (the delayed neutrons have a "softer" spectrum and thus have a different, usually smaller, leakage rate and capture rate)
- β_{eff} = total delayed neutron fraction
- k_{eff} = effective neutron multiplication factor (corrected for leakage)
- l = effective neutron lifetime (corrected for leakage)
- i = group index number
- N_n = number of delayed neutron precursor groups

^{†††}This relationship is calculated from the results of evaluating the variation of the k_{eff} with different diameters of fissile material in the pores of the tuff and the thermal history calculated from various diameters fissile material as discussed in Section 5.5.1 and shown in Figure 10-6.

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- λ_i = delayed neutron decay constant for precursor group i
 C_i = delayed neutron precursor concentration for group i
 q_n = additional neutron source

Rate of Neutron Population Increase. For a reactor operating at steady-state, the effective multiplication factor is unity (an increase in power corresponds to k_{eff} greater than unity and a decrease in power corresponds to a k_{eff} less than unity). The difference of the effective multiplicity from unity (steady-state) is:

$$\Delta k_{eff} = k_{eff} - 1 \quad (10-14)$$

The relative change (ratio of excess multiplication factor to effective multiplication factor) is:

$$\rho = \frac{\Delta k_{eff}}{k_{eff}} = \frac{k_{eff} - 1}{k_{eff}} \quad (10-15)$$

Because Δk_{eff} represents the increase of neutron population (per neutron generation), the rate of neutron population increase is given by:

$$\frac{dn(t)}{dt} = \frac{n(t)\Delta k_{eff}}{l} \quad (10-16)$$

The solution, for a constant Δk_{eff} is given by:

$$n(t) = n_0 e^{\frac{\Delta k_{eff}}{l} t} = n_0 e^{\frac{t}{T}} \quad (10-17)$$

where,

$$T = \frac{l}{\Delta k_{eff}} = \text{reactor period (i.e., } e - \text{folding time)} \quad (10-18)$$

Reactor Period. The reactor period is the time for the reactor to increase neutron population and hence power by a factor of e . Thus for a reactor with a neutron lifetime of 10^{-3} seconds and a k_{eff} of 1.005, the reactor would see a power increase of 148 times every second (i.e.,

$$\frac{n(t = 1 \text{ second})}{n(t = 0)} = e^{\frac{1.005 - 1}{10^{-3}}} = e^5 = 148.4 \quad (10-19)$$

thus this k_{eff} corresponds to a very high multiplication value). However, the effect from delayed neutrons means that the small number of delayed neutrons profoundly bias the average ("effective") neutron lifetime in the reactor system. Grouping the delayed neutrons is shown in Table 10-22.

The term β_i in Table 10-23 corresponds to the fraction of neutrons in a group and β is the total fraction of delayed neutrons (this is sometimes denoted as β_{eff} — the "effective" fraction of delayed neutrons). Thus $(1 - \beta)$ is the fraction of prompt neutrons. Likewise, the effective neutron lifetimes can be calculated by noting that:

$$l = \frac{\sum_{i=0}^{n_g} \beta_i(\%) l_{mean i}}{\sum_{i=0}^{n_g} \beta_i(\%)} = \frac{\sum_{i=0}^{n_g} \beta_i(\%) l_{mean i}}{100\%} \quad (10-20)$$

Table 10-22. Neutron Groups from Thermal Fission (1)

Group i	Half-Life for ^{235}U Fission $\tau_{1/2}$ (seconds)	Percentage of Thermal Neutrons from Fission		
		^{235}U ($\beta_i(\%)$)	^{239}Pu (2) ($\beta_i(\%)$)	
0	10^{-3}	99.359	99.790	Prompt neutrons
1	55.72	0.021	0.007	Delayed neutrons
2	22.72	0.140	0.063	Delayed neutrons
3	6.22	0.126	0.044	Delayed neutrons
4	2.30	0.253	0.069	Delayed neutrons
5	0.61	0.074	0.018	Delayed neutrons
6	0.23	0.027	0.009	Delayed neutrons
$\beta = \frac{\sum_{i=1}^{n_g=6} \beta_i(\%)}{\sum_{i=0}^{n_g=6} \beta_i(\%)} = \frac{\sum_{i=1}^{n_g=6} \beta_i(\%)}{100\%} =$				
		0.00641	0.00210	

(1) Source - Foster and Wright, 1977.

(2) ^{239}Pu values are also shown for comparison.

Thus taking into account the delayed neutrons, the power increase per second from Equation 10-20 should be 1.061 (versus 148 when only prompt neutrons are considered). Should the product of the multiplication factor and the fraction of prompt neutrons (i.e., $k_{\text{eff}} (1 - \beta_{\text{eff}})$) become equal to or greater than unity, then the reactor kinetics is governed by the neutron lifetime of prompt neutrons only (the delayed neutrons are no longer needed to sustain the nuclear chain reactions). This condition means that the growth rate of the power will be so large that the reactor may not be controllable by ordinary reactor control rod mechanisms. Thus, for very large reactivity increases ($\rho \geq \beta_{\text{eff}}$) the time scale of the prompt neutrons tends to dominate and the reactor is said to be prompt supercritical (see Table 10-24). Reactivity is often quantified in terms of fractions of β_{eff} , where reactivity is said to be worth one dollar when $\rho = \beta_{\text{eff}}$ (likewise, $\rho_{\$} = 10\%$ when $\rho = 0.10 \beta_{\text{eff}}$).

During a supercritical excursion, the power and temperature will rise until feedback effects become large enough to reduce the multiplication effects to a subcritical condition. The most important negative temperature feedback effects are: (1) density decrease (important for metal systems, in which the neutron leakage from the assembly is increased), (2) Doppler effects (broadening of resonance cross sections may be important to the reduction of the neutron multiplication), and (3) thermal expansion (this expansion with or without voiding or boiling, is the major feedback mechanism for solution systems). If supercriticality cannot be counteracted by these negative feedback effects, the assembly would break apart or melt (for metal assemblies) or disassemble by splashing or boiling (solution systems). The most conservative of these would be the rapid disassembly/vaporization of a metal assembly which can be analyzed by the Bethe-Tait method (see Bethe and Tait, 1956; Meyer et al., 1967; and Hetrick, 1971). This conservative method is appropriate only for systems that have a rapid positive reactivity insertion of substantial magnitude.

Table 10-23. Neutron Lifetime (Thermal Fission)*

Group i	$\beta_i(\%)$	Mean Lifetime		
		$l_{mean i}$ (seconds)	$\beta_i(\%)l_{mean i}$ (seconds)	
0	99.359	10^{-3}	0.09936	Prompt neutrons
1	0.021	80.40	1.688	Delayed neutrons
2	0.140	32.79	4.591	Delayed neutrons
3	0.126	9.01	1.135	Delayed neutrons
4	0.253	3.32	0.840	Delayed neutrons
5	0.074	0.88	0.065	Delayed neutrons
6	0.027	0.33	0.009	Delayed neutrons

$$\sum_{i=0}^{n_g=6} \beta_i(\%) = 100\%$$

$$l = \frac{\sum_{i=0}^{n_g=6} \beta_i(\%) l_{mean i}}{\sum_{i=0}^{n_g=6} \beta_i(\%)} = \frac{8.428}{100} = 0.0843 \text{ (seconds)}$$

* Source - Foster and Wright, 1977.

Table 10-24. Reactivity Insertion

$\rho < 0$	$k < 1$	subcritical (zero or decreasing power)
$\rho = 0$	$k = 1$	critical (could be at any power level)
$\rho > 0$	$k > 1$	supercritical (increasing power)
$\rho \geq \beta$	$k > \left(\frac{1}{1-\beta} \right)$	prompt supercritical (increasing power, dominated by prompt neutrons)

The reactor dynamics equation can be rewritten in terms of ρ and β as:

$$\frac{dn}{dt} = \frac{(\rho - \gamma\beta)}{l_g} n + \sum_{i=1}^{N_d} \lambda_i C_i + q_n \quad (10-21)$$

where:

$$l_g = \frac{l}{k_{eff}} = \text{neutron generation time} = \text{total cycle time} \quad (10-22)$$

Total Neutron Lifetime. The total neutron lifetime is the sum of the slowing down time (l_s , the time that it takes for the fission produced high energy neutron to slow down to thermal energies) and the thermal lifetime (l_{th} , the time

that the thermal neutron spends diffusing at thermal energies before sorption). The slowing down time is very short (for a pure moderator material the slowing down time is roughly two orders of magnitude less than the thermal lifetime) and the neutron lifetime is dominated by the thermal lifetime, thus

$$l = l_{th} + l_s \approx l_{th} \quad (10-23)$$

Typical neutron lifetimes are shown in Table 10-25 for pure moderator materials. For mixtures that include uranium or plutonium, the neutron lifetime is much less due to increased neutron sorption in these metals. (The neutron lifetime for a neutron in a typical thermal reactor is about 10^{-3} seconds.) It can thus be seen that the selection of moderator material can greatly affect the reactor dynamics.

Table 10-25. Neutron Lifetimes in Pure Moderator Materials

Moderator	Slowing Down Time (seconds)	Thermal Lifetime (seconds)
C	1.5×10^{-4}	1.8×10^{-2}
H ₂ O	5.6×10^{-6}	2.1×10^{-4}
D ₂ O	4.3×10^{-5}	1.4×10^{-1}
Be	5.7×10^{-5}	3.7×10^{-3}

The equation which describes the time rate of change of the concentration of delayed neutron precursors is given by:

$$\frac{dC_i}{dt} = \frac{\gamma_i \beta_i k_{eff}}{l} n - \lambda_i C_i \quad (10-24)$$

$$\left\{ \begin{array}{l} \text{time rate} \\ \text{of change of} \\ \text{precursors} \end{array} \right\} = \left\{ \begin{array}{l} \text{precursor} \\ \text{production} \\ \text{rate} \end{array} \right\} - \left\{ \begin{array}{l} \text{precursor} \\ \text{loss rate} \end{array} \right\} \quad (10-25)$$

where,

- C_i = delayed neutron precursor concentration for group i
- λ_i = the decay constant for C_i
- γ_i = the group i energy correction factor

Correcting β for the energy spectrum of the neutron flux yields:

$$\gamma\beta = \sum_{i=1}^{N_g} \gamma_i \beta_i \quad (10-26)$$

Reformulating the equation in terms of l_g yields:

$$\frac{dC_i}{dt} = \frac{\gamma_i \beta_i}{l_g} n - \lambda_i C_i \quad (10-27)$$

Equations 10-20 and 10-26 are solved to obtain the time dependent values for the neutron population (which can be used in calculating the instantaneous reactor power) and the delayed neutron precursor concentrations. For gen-

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eral cases, only neutron groups are used (see Table 10-22). Also required for a reactor system analysis is the decay heat precursor concentrations. They are evaluated by

$$\frac{dH_j}{dt} = \beta_j^H n - \lambda_j^H H_j \quad (10-28)$$

where,

H_j = group j decay heat precursor concentration

β_j^H = group j decay heat fraction

λ_j^H = decay constant for decay heat precursor group j

The decay heat power is then given by

$$n_h = \sum_{j=1}^{N_h} \lambda_j^H H_j \quad (10-29)$$

where,

N_h = the number of decay heat precursor groups
(this is not necessarily the same as N_n)

The prompt neutron power (fission thermal power) is given by

$$n_p = (1 - \beta^H) n \quad (10-30)$$

where the total decay heat fraction is given by,

$$\beta^H = \sum_{j=1}^{N_h} \beta_j^H \quad (10-31)$$

Typical values of β^H are in the neighborhood of 0.07 (unlike β , which is ~ 0.007 , see Tables 10-22 and 10-26).

The effective reactor thermal power is thus expressed as:

$$n_e = n_p + n_h \quad (10-32)$$

The above equations yield two parameters for total power: (1) n (the total instantaneous neutron power) and (2) n_e (the effective thermal power). The first, n , would be that determined from neutron detector measurements. The second, n_e , is the power that be transferred to the coolant and correspondingly result in the coolant temperature rise. These parameters are equal only at equilibrium conditions.

System Reactivity and Precursor Concentrations. Initial values for the system reactivity and the precursor concentrations (delayed neutron and decay heat) are given by:

$$\rho^0 = \gamma\beta - l_g \left(\frac{\sum_{i=1}^{N_n} \lambda_i C_i^0 + q_n^0}{n^0} \right) \quad (10-33)$$

Table 10-26. Delayed Heat Precursor Constants for ^{235}U (*)

Group i	Decay Constant for ^{235}U Fission λ_j^H (sec $^{-1}$)	Decay Heat Precursor Fractions for ^{235}U Fission	
		(β_j^H)	
1	1.772	0.00299	Delayed neutrons
2	0.5774	0.00825	Delayed neutrons
3	0.06743	0.0155	Delayed neutrons
4	0.006214	0.01935	Delayed neutrons
5	4.739×10^{-4}	0.01165	Delayed neutrons
6	4.81×10^{-5}	0.00645	Delayed neutrons
7	5.344×10^{-6}	0.00231	Delayed neutrons
8	5.726×10^{-7}	0.00164	Delayed neutrons
9	1.036×10^{-7}	0.00085	Delayed neutrons
10	2.959×10^{-8}	0.00043	Delayed neutrons
11	7.585×10^{-10}	0.00057	Delayed neutrons
$\beta^H = \sum_{j=1}^{N_H=11} \beta_j^H =$		0.06999	

* Source - ANS, 1971.

$$C_i^0 = \frac{\gamma_i \beta_i}{l_g \lambda_i} n^0 \quad (10-34)$$

$$H_j^0 = \frac{\beta_j^H}{\lambda_j^H} n^0 \quad (10-35)$$

The coupling of the reactor dynamics to the thermal-hydraulics is done through the total reactivity (ρ). The thermal-hydraulics code uses the effective thermal power to calculate the thermal response of the repository system (including the inner reactor-type assembly). The resultant geometry, i.e., movement of water moderator, system temperature profiles) is then used at each instance in time to determine the reactivity. As the system heats up and decreases saturation in or near the inner reactor-type region, the reactivity decreases. This self shutdown mechanism is the feedback relationship between the thermal-hydraulics and the reactor dynamics physics. The important features of the system behavior are: (1) the integrated amount of energy release per each excursion and (2) the system recovery time (the duration of time for conditions to return to a criticality geometry), which yields the maximum spatial excursion frequency.

Table 10-27. Delayed-Neutron Half-Lives, Decay Constants and Yields from Thermal Fission (1)

Group index, i	Half-life $\tau_{1/2}$, sec	Decay constant λ , sec ⁻¹	Relative abundance $a_i \equiv \frac{\beta_i}{\beta}$	Absolute group yield, %
²³⁵ U (99.9% ²³⁵)				
1	55.72 ± 1.28	0.0124 ± 0.0003	0.033 ± 0.003	0.052 ± 0.005
2	22.72 ± 0.71	0.0305 ± 0.0010	0.219 ± 0.009	0.346 ± 0.018
3	6.22 ± 0.23	0.111 ± 0.004	0.196 ± 0.022	0.310 ± 0.036
4	2.30 ± 0.09	0.301 ± 0.011	0.395 ± 0.011	0.624 ± 0.026
5	0.610 ± 0.083	1.14 ± 0.15	0.115 ± 0.009	0.182 ± 0.015
6	0.230 ± 0.025	3.01 ± 0.29	0.042 ± 0.008	0.066 ± 0.008
²³⁹ Pu (99.8% ²³⁹) (2)				
1	54.28 ± 0.54	0.0128 ± 0.0005	0.035 ± 0.009	0.021 ± 0.006
2	23.04 ± 1.67	0.0301 ± 0.0022	0.298 ± 0.035	0.182 ± 0.023
3	5.60 ± 0.40	0.124 ± 0.009	0.211 ± 0.048	0.129 ± 0.030
4	2.13 ± 0.24	0.325 ± 0.036	0.326 ± 0.033	0.199 ± 0.033
5	0.618 ± 0.213	1.12 ± 0.39	0.086 ± 0.029	0.052 ± 0.018
6	0.257 ± 0.045	2.69 ± 0.48	0.044 ± 0.016	0.027 ± 0.010

(1) Total data for each fission nuclide were obtained from 40 prompt-burst irradiations and 40 saturation irradiations. Isotopic purity of fission sample is indicated in parentheses. Data taken from Keepin, (1965).

(2) ²³⁹Pu values are also shown for comparison.

10.7 Findings and Recommendations

10.7.1 Summary of Findings

To roughly estimate the probability of a criticality occurring, the circumstances within the four types of criticalities, the design features of the containers, the orientation of waste emplacement, and the repository layout were combined in a fault tree. The fault tree assumed that enough water to create a criticality might be introduced as the result of a climatic change and subsequent percolation through connecting cracks or "weeps" in the tuff. Based on this study, a water-moderated criticality involving at least one waste container over a duration of 10,000 yr had a probability above 10^{-4} (Table 10-28). Because water is essential for producing conditions conducive to a criticality by significantly changing the container, allowing assembly of the fissile material, and possibly moderating the nuclear reaction, the probability assigned to climatic change and subsequent percolation is crucial in the fault tree.

The preliminary finding that the probability of a criticality event could not be readily dismissed led to (a) studies bounding the consequences and (b) a much more detailed evaluation of the criticality that included processes that are required to more fully understand a criticality occurrence within a repository. The bounding analysis showed that consequences would be minimal.

Specifically, bounding calculations revealed that a local moderated, low rate of critical assembly produces no more than 10^{25} fissions during 10,000 yr. Assuming a 12,060 MTHM repository of spent fuel with an average burnup of between 25,000 and 40,000 MWd/MTHM, the number of fissions that is represented by the spent fuel is on the order of 10^{30} fissions (see Volume 3, Appendix A). Consequently, an increase in the inventory of fission products from one critical event of 10^{18} fissions is negligible; only those radionuclides with very short half-lives have an appreciable increase in comparison to the original inventory. Similarly, the impact of 10^{25} atoms split from a critical condition occurring in a container in the repository, assuming a steady-state reactor, is still negligible. Furthermore, if one assumes that 289 MPCs with highly enriched uranium spent fuel all go critical, about 10^{28} fissions occur, which is only 1% of the inventory when represented as fissions for a 12,060-MTHM repository with 25,000 to 40,000 MWd/MTHM burnup (Table 10-28).

Although the consequences are minor from this conceptualization, it was not based on interplay of all pertinent phenomena. Indeed, the most important feature of the criticality condition is determining likely initial conditions. For example, another analysis with different, and improbable, starting conditions might generate results that incorrectly indicate large nuclear excursions. Thus, it is imperative to understand how fissile mass might assemble in a repository and then examine the interplay of controlling parameters such as water saturation, power output, and temperature. Consequently, these factors were studied in the 1994 PA.

Table 10-28 summarizes the information gathered about critical conditions in or near containers.

Also, during the final phase of the development of this chapter, some very significant findings substantially changed the perception of the mechanisms that might result in a "criticality" excursion in a tuff repository. However because of time constraints, this chapter was not substantially altered to explicitly reflect this information. The newer information is preliminary (physical insight should be focused upon trends and not the exact numbers calculated). Stated briefly, the new information is provided below:

Even though it is not possible to predict the probability and/or location of a far-field critical mass, calculations were performed to investigate the consequences of a "criticality excursion." These calculations correspond to the "nuclear dynamics" of the system. Ideally, the nuclear dynamics would correspond to the coupling of the nuclear kinetics (time behavior of a nuclear assembly) to the transient geologic (two-phase) thermal/hydraulics. The complete dynamics model would include the feedback mechanisms (such as desaturation and temperature feedback coefficients) that would identify self-shutdown mechanisms of the nuclear chain reactions. Initial criticality (steady-state) calculations to determine the feedback worths of desaturation mechanisms indicated that k_{eff} , the multiplication factor, is very sensitive to the groundwater saturation.

Table 10-28. Summary of Information Gathered about Critical Conditions in or Near Containers

Consequences of Critical Conditions assuming High Moderation and Low Reactivity

1. A steady-state reactor limited to 1 kW (~ 1 mg ^{235}U) to prevent boiling of water in a container would generate about 10^{25} fissions over 10,000 yr.
2. The percentage increase in the total inventory and the inventory of most of the radionuclides from fission, should one container go critical and produce 10^{25} fissions (similar to documented aqueous accidents) over 10,000 yr, is insignificant. Even 10^{28} fissions in about 289 containers with highly enriched uranium would be only 1% of the $\sim 10^{30}$ fissions represented by a 12,060 MTHM repository containing spent fuel with burnup of 40,000 MWd/MTU.
3. Using a 2-phase flow composite-porosity model and assuming 100% water saturation of between 1 and 10 kg of fissile material, the forced startup of a natural reactor would potentially operate for between 1 and 1000 days (for 10^{21} and 10^{19} fissions, respectively) before the water saturation dropped by 15%. The system took between 70 and 200 days to recover to 99% saturation.
4. In the slow fission process envisioned to occur in a repository, gaseous fission products such as ^{85}Kr (with the longest half-life of 10.78 yr) decay more rapidly than they are transported to the regulated boundary in the first 500 yr, but could escape after 1000 yr (see Figure ES-9). However, diffusion into the atmosphere would greatly diminish the doses.
5. The effect of additional heat generation from a criticality condition on regional liquid flow is also insignificant.

Probability of Critical Conditions

6. A preliminary fault tree analysis showed that the possibility of a critical event could not be readily dismissed (ignored as a scenario).
7. Assuming a composite-porosity model with climate change, concentration of the infiltration, and the disposal containers of 20-mm Incoloy Alloy 825 and 100-mm carbon steel, a median value of 30 and a mean of 700 kg of fissile material would be transported from all 475 MPCs containing spent nuclear fuel within 10,000 yr.
 - Assuming only 289 containers with large amounts of fissile material, the deposition region near a container would hold between 0.1 and 2.4 kg of fissile material.
8. The operation of a natural *unpressurized* waste reactor is extremely sensitive to water saturation. Because k_{eff} is changed by any slight change in saturation, the nuclear chain reaction is immediately shut down.
 - Using the assumptions of these preliminary nuclear dynamics calculations, a large pressure rise is not feasible in a partially saturated, unpressurized natural reactor because of the sensitivity of k_{eff} to the saturation.
9. Between 10^1 to 10^7 times more ATR uranium metal than borides (e.g., chromium-boride) is altered inside containers.

Because a Monte Carlo computer code was used for the k_{eff} computations, the stochastic errors for k_{eff} were too large to permit fully coupling of a point kinetics model to the thermal/hydraulics model. Instead, a series of uncoupled modeling was attempted. (In the uncoupled form, the dynamics modeling can be estimated by alternately performing kinetics calculations and then thermal/hydraulics calculations, iterating the process until an acceptable level of accuracy is achieved.) Even this approach proved to be problematic in that should a critical mass be assembled and any meaningful amount of heat be generated, which would result in a slight amount of desaturation of groundwater, the corresponding negative power feedback coefficient of the assembly would very rapidly shut down the nuclear chain reactions and the power of the system. The self-shutdown mechanisms are so sensitive to the groundwater saturation (a desaturation of 1% by volume has a corresponding reactivity decrease of -0.31 [minus 31 cents]) that it was not possible to generate a nuclear excursion with an integrated fission release anywhere near that reported in the literature for aqueous criticality accidents that had occurred in the past at processing plants.

Thus, to investigate the effects of large excursions, several excursion sizes (10^{19} , 10^{20} and 10^{21} integrated fissions per excursion) were forced to occur. These excursion sizes could not physically occur, but were used to interrogate the response of the geological system. This simulation was done by forcing one of these large excursions to

occur and then identifying the amount of time that it took for the geological system to recover to the initial groundwater saturation conditions. The identified recovery (cycling) time and the fission release per event were then used to determine the total fissions that occurred during the 10,000-yr regulatory period. The obtained results indicated that the radionuclides added to the inventory due to the added criticality excursions were insignificant in comparison to the initial radionuclide inventory.

At present, the only other known nuclear dynamics modeling of fissile/geological system was for the Oklo phenomenon (Bilanovic, 1985; Kuroda, 1990). These attempts did not compare with one another and failed to include any thermal/hydraulics modeling because of the lack of geologic hydrology data. (The Oklo deposits were completely mined out before it was identified that sixteen independent critical assemblies had occurred in that location.) Even if Oklo phenomenon nuclear dynamics models or calculations were available, they would not be useful for this project because the Oklo site corresponded to a pressurized system. The most important findings identified in this preliminary nuclear dynamics modeling in the 1994 PA were that should a critical assembly be formed in a geological repository, the feedback control mechanisms are highly negative and, even more important, the integrated fissions are not significant.

Auto-Catalytic Criticality Excursion. Of recent concern has been the discussion amongst the geological repository community of the possibility of a dry silica oxide-moderated system that could experience an auto-catalytic criticality excursion. Although, silica-oxide (or silica-dioxide) has the classical characteristics of a moderator (the dependence of k_{eff} upon the moderator/fissile atom ratio), it is a very inefficient moderator and massive masses of fissile material are required to generate a critical assembly. The isolation of such large masses of fissile material would require significant volumes of groundwater to either transport neutron absorbers away from the fissile assembly or to transport fissile material to an assembly location. (Even more important, the postulated scenario started with an initial condition that was highly supercritical.) In either case, the geological processes that would be needed to yield the initial critical system would induce self-shutdown mechanisms identified in the 1994 PA; thus, it would not be plausible to develop a highly supercritical dry moderated system. However, several features (such as Doppler broadening) of the dry silica oxide-moderated system may warrant some future investigation to insure that this type of feature is not of concern.

10.7.2 Recommendations

Except for the performance assessment, few other engineering/scientific studies of the consequences of a repository criticality have been completed. Based on the information currently available, it appears that a criticality is not disruptive to the performance of a geologic repository for either commercial or highly enriched spent fuel. However, additional efforts directed toward risk assessment, including criticality calculations and performance assessments, will be necessary.

First, little work has been done to establish repository post-closure criticality safety requirements and policy. Thus, there is not as yet a consistent or coherent approach to what technical (risk-based) assumptions can or should be applied in a criticality. A plausible set of repository conditions needs to be established with respect to any proposed criticality scenario. Furthermore, methodologies necessary to deal with technical analysis and evaluations (PAs) assignment of risk quantification, probabilistic risk assessments, and criticality calculations need some degree of standardization. Because commercial-type fuel and highly enriched spent fuel have many characteristics in common, cooperative efforts between Office of Environmental Management (DOE-EM), which is responsible for the DOE spent fuel, and the Office of Civilian Radioactive Waste Management (DOE-RW), which is responsible for commercial spent fuel, could be mutually beneficial.

Second, validation of repository criticality calculations remains to be completed and awaits development of applicable data. In general, the computer programs used for criticality safety calculations require verification, usually by comparison of calculated results with experimental data that represent the conditions of the system being modeled. A number of criticality safety programs (SCALE, MCNP, and others) have been extensively verified under conditions typical of fuel reprocessing or fuel storage. In applying these programs to repository criticality calculations, conditions are different enough from fuel reprocessing and fuel storage conditions to introduce uncertainty. Conservative

assumptions can accommodate most uncertainties, but not necessarily all. Therefore, some type of experimental data representative of repository conditions (unavailable as yet) are needed to fully validate the repository criticality calculations that have and will be made.

Third, a key analysis area that needs additional study is to examine the corrosion and leaching of borated stainless steel (or other borated material) versus the removal of uranium. Although some calculations were done, a detailed analysis of the corrosion of borated stainless steel in the canister inner baskets was not possible given the scope of the 1994 PA. This modeling is necessary to identify whether borated material is leached away from a canister over a 10,000-yr period in amounts substantial enough to be of concern. (Initial calculations indicated that uranium migrated before the boron; see Section 10.5.4.) Included in this work would be an analysis to determine the solubility of boron in the tuff groundwater and corresponding material transport.

Although much was accomplished in the 1994 PA with regard to criticality, future studies need to perform more calculations to adequately model processes that would create conditions conducive to a criticality within the repository and its consequences. A key analysis area that needs additional study is to examine the corrosion and leaching of borated stainless steel (or other borated material) versus the removal of uranium. Although some calculations were done, a detailed analysis of the corrosion of borated stainless steel in the canister inner baskets was not possible given the scope of the 1994 PA. This modeling is necessary to identify whether borated material is leached away from a canister over a 10,000-yr period in amounts substantial enough to be of concern. (Initial calculations indicated that uranium migrated before the boron; see Section 10.5.) Included in this work would be an analysis to determine the solubility of boron in the tuff groundwater and corresponding material transport. Initially, this modeling should examine more uncoupled events to develop an understanding of the feasibility of the critical event in a moderated but unpressurized assembly of fissile material before coupling currently existing nuclear reactor, lumped-parameter codes with current two-phase flow codes to evaluate dynamics of critical conditions. This analysis can first continue to examine more of the conditions and assumptions hypothesized in the fault tree for criticality event in or near a waste container. However, a coupling of fluid flow and nuclear physics can be done without much more effort and should also be attempted because the end result may be more informative.

While the probability of assembling large amounts of fissile material is low, future studies should perform scoping calculations to examine assemblies with larger amounts of fissile material than were used in the 1994 PA to see whether sensitivity to minute changes in saturation is reduced.

Because the assembly of sufficient fissile material and water for moderation is difficult in the geologic setting, the addition of a few features in the container or repository could further reduce the probability of a critical condition. Hence, future studies should examine potential options to lower the probability of critical conditions occurring within the repository such as adding filler (internal backfill) within the container to reduce the volume of water available to moderate nuclear reactions.

An additional area is to examine the possibility and consequences of a critical condition at the surface after an exploratory borehole has penetrated the repository and brought fissile material to the surface. Because bringing fissile material to the surface already represents a release, this situation was not examined in the 1994 PA. However, the critical event should probably be quantified to some extent such that the additional hazards from a criticality can be compared to the hazard of releasing the contents of a spent fuel container at the surface.

A final area to be explored is to develop the capability to model precipitation of fissile material in transport calculations. Incorporating this capability into current models would be relatively easy; the more difficult aspect would be constructing numerical models with fine grids, yet reasonable run times, and the proper correlation of solubilities within and outside the container.

11. Parcel Corrosion and Source Term Models

C. T. Stockman, M. A. Martell, and J. S. Rath

Two submodels, GASSNF and CONCSNF, were written for the 1993 PA to model the corrosion of waste parcels and the resultant release of radionuclides. These models were written for a saturated environment where corrosion was dominantly anoxic and water was the limiting reactant for the corrosion reactions. Due to the controlling nature of the water/gas budget, the GASSNF modeling focused on the consumption of water and production of gas from the corrosion process, as well as the breach of the successive layers of protection for the radionuclides. No attempt was made to model the transport of radionuclides through breaches in the parcel layers in CONCSNF, but instead an assumption was made that a failed parcel offered no transport resistance. Transport of radionuclides up the borehole through the bentonite backfill was not modeled by CONCSNF but left to the transport codes to calculate.

The 1994 PA differs from the 1993 PA in several important areas. The repository chosen for study is unsaturated and expected to be somewhat oxic. Water is the limiting reactant, but acts as a medium or catalyst for the oxidation of the waste parcels. The parcels are not set in backfill, but emplaced with an air gap between them and the host rock. Also, 10 CFR 60 and dose calculations to 100,000 yr in addition to 40 CFR 191 were used to measure compliance. Because of these differences, GASSNF required some enhancements. The changes needed in CONCSNF were significant enough that the source term model was renamed USATCONC, for unsaturated concentration. This chapter discusses GASSNF and USATCONC, the processes of parcel degradation and radionuclide release, and how these processes were modeled. These models were used in both the Simple and Complex PAs (Chapters 12 and 13). An understanding of these models will be beneficial in interpreting the results.

11.1 Gas Generation/Parcel Corrosion Submodel, GASSNF

GASSNF is a collection of FORTRAN routines that model the corrosion and breach (penetration) of the nested layers of containment provided by waste emplacement parcels. The models allow for any number of waste parcels and mixtures of waste parcels to be defined by the user. The design of the waste parcels is entered into a database as a series of layers with associated composition, surface area, and mass as shown in Chapter 4. The assignment of waste parcels to individual grid locations is accomplished in an input file by the analyst after the calculational mesh is created.

11.1.1 Contact with Groundwater – Container Groups

The emplacement scheme modeled in the 1994 PA provides for separation of the parcel from the host rock. This separation is achieved through emplacement of the parcel either on a stand or a railroad car and the inclusion of an air gap between the parcel and the host rock. This air gap serves two purposes: it provides for good radiative heat transfer from the waste parcel to the host rock, and it provides a capillary break so that groundwater will not be in contact with the parcel unless the host rock flow or saturation increases to a point where dripping occurs or much less likely, the repository is flooded. Because the integrity of the drift walls and ceiling cannot be totally ensured during the regulatory period, an assumption is made that some fraction of the waste parcels will come in contact with host rock rubble and thus in more intimate contact with groundwater (Figure 11-1). To account for this variation in water contact in the 1994 PA, the parcels were modeled in at least two groups: parcels with an intact air gap, and parcels with rubble bridging the air gap.

In the 1993 PA, all parcels were emplaced with a bentonite backfill so their mode of contact with water was constant. Two groups were used so that parcels with defects or emplacement damage could be modeled as well as the "normal" parcels. For the 1994 PA, the structure of GASSNF was generalized so that additional criteria for dividing the parcels could be easily added. Two criteria that were implemented in the calculation were the integrity of the parcel and the integrity of the air gap. The resulting container groups are shown in Table 11-1.

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Figure 11-1. Waste parcels in contact with host rock rubble.

Table 11-1. Container Groups for 1994 PA

Container Group	Good Parcel	Good Air Gap
1	yes	yes
2	no	yes
3	yes	no
4	no	no

Two water contact modes were included in GASSNF and their effects on parcel corrosion were modeled. It is generally accepted that at low temperatures, wet corrosion is much faster than humid corrosion. In fact, some experiments show that in an irradiated unsaturated tuff environment, the fastest corrosion occurs when the canisters are damp (Yunker and Glass, 1987). Yunker and Glass suggest that the fast corrosion rate was a result of the nitric acid and various other oxides of nitrogen, created by radiolysis of air, dissolving into the thin film of water condensed on the container. They suggest that damp conditions resulted in the highest concentration of nitric acid on the metal surface because the high fraction of air provided the most NO_x from radiolysis and the thin film of water kept dilution to a minimum. This effect, however, would be difficult to model since the phenomena have not been well quantified, and it is not clear that condensation will occur on canisters within a repository as they did in Yunker and Glass' experiments. Both the capillary draw of the host rock and the higher temperatures of the waste parcels will tend to prevent condensation onto the parcels, at least at early times. As corrosion products build up on the parcels, causing their own capillary draw and boiling point elevation and as the parcels cool off, condensation will become more likely. For simplicity, condensation as a water contact mode was not modeled in the 1994 PA; instead, uncertainty was included in the corrosive nature of the groundwater during assignment of ranges of the wet corrosion rates.

Models used in the 1992 PA for the WIPP (WIPP PA Department, 1992b) used wet and humid corrosion rates and a weighted average of the two based on the grid block saturation. This method is appropriate for transuranic waste that spans several grid blocks but was deemed inadequate for the 1993 PA calculations. The first method tried in the scoping calculations for the 1993 PA was to use a moist corrosion rate (0) when the grid block saturation fell below residual, and a wet corrosion rate when the saturation was above residual. (Residual saturation is defined as the saturation below which water does not undergo darcy flow—see Chapter 12.) The rationale for this approach was that if the region immediately surrounding the canister becomes dry due to consumption of water in the corrosion process, water will be replaced by capillary draw if the grid block is above residual saturation, but will not be replaced if the grid block is below residual saturation. This step function was found to cause numerical instability in the BRAGFLO_T code, so an exponential function that approximated a step function was used.

For the 1994 PA, the two most likely modes of water contact considered were dripping when the air gap is intact, and capillary draw when there is rubble in contact with the waste parcel. For the intact air gap case, no dripping occurred as long as the tuff matrix was able to carry the fluid flow and the fractures were below residual saturation. When the fractures were above residual saturation, however, they would be flowing and they could drip on the waste parcels. We decided to use the same function as used in the 1993 PA, to approximate a step function that would turn wet corrosion off if the fracture saturation fell below residual. No claim is made that this function accurately describes the dependence of canister corrosion on the saturation and flow within a tuff repository. For example, if condensation were a major factor in water transport to the canisters, this function would be wrong. This function is included as an attempt to show some of the dependence that is expected, but it is left to future researchers to establish a defensible function for this phenomenon. The same equation was used for the case of rubble around the parcel, but wet corrosion was allowed to occur until the saturation in the fracture was zero. Because it is desirable in PA calculations to have models that are defensibly conservative when phenomena are not well parameterized, a simple model for the moisture dependence of corrosion rates was also included in GASSNF. When the user selects this option, the full corrosion rate is used whenever the waste parcel (WP) or grid block temperatures are below the boiling point. This option was used in the scoping calculation only.

11.1.2 Types of Corrosion

As in the 1993 PA, two types of corrosion are modeled, generalized (uniform) and localized (any non-uniform corrosion such as pitting and stress corrosion cracking). Uniform corrosion is emphasized in GASSNF because of its importance in overall gas and water consumption/production, as well as its role in the penetration of materials such as carbon steel. For materials such as Incoloy Alloy 825, localized corrosion is more important than uniform corrosion because it results in rapid penetration. The localized corrosion is once again specified by the input parameter "FRCPEN" which is defined as the fraction of mass of a layer corroded at the time of penetration of that layer, with a FRCPEN of 1 indicating no localized corrosion and a FRCPEN of 0 indicating that the layer is penetrated before any generalized corrosion occurs.

In the 1993 PA, GASSNF modeled only anoxic corrosion, which was expected to be the dominant process in the saturated repositories. In an unsaturated tuff repository, wet oxic and humid oxic corrosion are also needed so GASSNF was generalized to allow as many corrosion types as necessary. The parameters for three corrosion types have been input into the database, using the two letter suffixes wo, ho and wa to denote wet oxic, humid oxic, and wet anoxic. (Humid anoxic corrosion is expected to be negligible.) Because oxidation of a metal is usually dependent on the oxygen fugacity of the gas or liquid phase in contact with it, the inclusion of a term that would show such a dependence was desirable. This idea, however, was presented to the BRAGFLO_T and NUTS code developers too late in the code revision cycle for them to add transport of oxygen. Consequently, BRAGFLO_T modeled only the gas phase transport of water vapor and "air." Oxygen consumption or hydrogen production by GASSNF was handled by BRAGFLO_T as "air" consumption/production. The only variable related to oxygen fugacity that would be available to the GASSNF code, would be x_{air} (the mass fraction of the gas phase that is "air," not water vapor), which is calculated by BRAGFLO_T. During heat up and boiling of the water around the repository, x_{air} was expected to decrease significantly as the air was displaced by water vapor. Therefore, we added x_{air} as a simple multiplier to the corrosion rate. When $x_{\text{air}} = 1$, the full corrosion rate as described in the literature is used. As the mass fraction of air is decreased by displacement with water vapor, the corrosion rate is decreased proportionately. Because proper treat-

ment of the oxygen concentration within the repository was not possible, a decision was made to follow the practice of earlier performance assessments of tuff and assume that the air flow through the fractured unsaturated tuff was fast enough to assure that the mole fraction of oxygen within the "air" portion of the vapor phase remained at 0.2 at all times. Because anoxic corrosion is generally slower than oxidic corrosion, the assumption of fast air flow makes modeling the anoxic corrosion modes unnecessary; therefore, only the wet oxidic and dry oxidic corrosion modes were included in the 1994 PA. In future calculations, the anoxic reactions may be easily added. The corrosion parameters used are provided in Section 11.3.4.

11.1.3 Equations for Generalized Corrosion

Three equations have been included in GASSNF to model uniform corrosion as described below. For each layer material, the user selects an equation to use by means of the input parameter CORMOD. (The corrosion parameters are listed in Section 11.3.4.)

Equation 1:

When CORMOD is set to 0, Equation 11.1.3-1 is used.

$$M = A \cdot e^{-B/T} \cdot (t_2^C - t_1^C) \cdot D \cdot E \cdot SA \quad (11.1.3-1)$$

where:

- M = mass of layer corroded in time step,
- A = Arrhenius-type pre-exponential term ($\text{kg/m}^2\text{s}$), input as COR_A_XX (Section 11.3) where XX is the two letter suffix WO, WA, or HO as described above,
- B = Arrhenius-type activation energy term (K), input as COR_B_XX,
- T = temperature of the layer (K), passed from the flow code or read from a time/temperature file for each waste parcel as output by CONRAD. (When the temperature dependence of the corrosion rate is unknown, term B is set to zero and the temperature term drops out of Equation 11.1.3-1.)
- t_2 and t_1 = time at the beginning and end of the time step in seconds,
- C = time dependence term, input as COR_C_XX,
- D = saturation dependence term,
- E = oxygen concentration dependence term,
- SA = surface area of the layer.

Many materials obey a parabolic or cubic time dependence equation, in that the rate of corrosion decreases as the thickness of a protective layer of corrosion products increases. These equations are usually expressed as functions of time although they should more accurately be expressed as functions of reaction progress when the reaction conditions are not constant. In the 1994 PA, corrosion of all layers does not start at time zero. Therefore use of the step times t_1 and t_2 in the time-dependent term is valid only for the humid corrosion of the overpack or for corrosion that is time invariant. Time invariant corrosion rates are indicated with a COR_C_XX of 1. Future work should redefine this term as a reaction progress term.

The saturation-dependent term, D, is either set to 0.0, 1.0 or Equation 11.1.3-2 for wet corrosion depending on a user input option and the waste parcel temperature. If the waste parcel temperature is above boiling, term D is set to 0. Equation 11.1.3-2 is an approximation of a step function that gives 0 up to a threshold saturation value and then 1.0 thereafter. The step function could not be used within BRAGFLO_T because it caused numerical instability. Equation 11.1.3-2 is plotted in Figure 11-2 using the parameters values (see Section 11.3) that were used for waste parcels with and without an intact air gap. For humid corrosion, term D is always set to 1.0.

$$D = 1 - e^{(-\alpha \cdot (\text{Sat} - \text{TS}))} \quad (11.1.3-2)$$

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Figure 11-2. Step function equation plotted with values for waste parcels with and without an intact air gap.

where:

- α = $\ln(.01)/(S_{99} - TS)$
- Sat = fracture water saturation,
- TS = threshold fracture saturation below which wet corrosion does not occur,
- S_{99} = fracture saturation where the wet corrosion rate is 99% of the corrosion rate at 100% saturation.

The oxygen concentration term, E, has been approximated by x_{air} , the mass fraction of air within the gas phase, in the 1994 PA. This term is intended to be changed to the mole fraction of the gas phase which is oxygen, when this information becomes available, at least for materials such as carbon steel which show a linear corrosion rate-oxygen fugacity dependence (Kirby, 1979).

Equation 2:

When the surface area of a material is difficult to estimate, such as the uranium carbide particles in the graphite spent fuel, the user may choose to use Equation 11.1.3-3 by setting CORMOD to 1.

$$M = A \cdot e^{-B/T} \cdot (t_2^C - t_1^C) \cdot D \cdot E \cdot M_{layer} \quad (11.1.3-3)$$

where A is now in units of 1/s and M_{layer} is the mass of the layer at time zero.

Equation 3:

The third corrosion equation (Equation 11.1.3-4) was included so that the corrosion equation for carbon steel used by Lamont could be selected. CORMOD = 3 selects this equation.

$$M = (AT^2 + BT + C) \cdot SA \quad (11.1.3-4)$$

where A, B and C are terms obtained from a quadratic fit to temperature-dependent corrosion data.

After equations are chosen, GASSNF calculates the corrosion rate for each corrosion type selected for the analysis (in this case wet oxid and humid oxid), and uses the maximum rate. For example, when the fracture saturation is above residual, and the waste parcel temperature is below boiling, the wet oxid corrosion rate is greater than the humid oxid corrosion rate, but when the fracture saturation is below the threshold saturation or the waste parcel temperature is above boiling, the wet corrosion rate goes to zero and the humid rate is used.

As in the 1993 PA version, GASSNF first calculates the mass of each layer that is corroded and then calculates the amount of water and gas that is produced or consumed by that process. It sums the water and gas produced or consumed by all exposed layers of all waste parcels in a grid block and divides this sum by the time step interval, which gives BRAGFLO_T the total gas and water production/consumption rates for each grid block. In addition, the new GASSNF also calculates a running total of the mass of rust (iron corrosion products) produced by each waste parcel for use by the source term model for sorption of radionuclides. For the generalized corrosion reaction:

where

$s_{\text{h}_2\text{o}}$ = the stoichiometry for water, moles water consumed per mole metal consumed,
 s_{gas} = the stoichiometry for gas, moles of gas produced per mole of metal consumed,
 s_{rust} = the stoichiometry for rust, moles of rust produced per mole of metal consumed,

(Note, this reaction was defined for an anoxic repository. In an oxid repository, $s_{\text{h}_2\text{o}}$ is usually zero and s_{gas} is usually negative.)

$$\begin{aligned} \Delta M_{\text{gas}} &= \Delta M_{\text{metal}} \cdot s_{\text{gas}} \cdot \text{MW}_{\text{gas}} / \text{MW}_{\text{metal}} \\ \Delta M_{\text{h}_2\text{o}} &= \Delta M_{\text{metal}} \cdot s_{\text{h}_2\text{o}} \cdot \text{MW}_{\text{h}_2\text{o}} / \text{MW}_{\text{metal}} \\ \Delta M_{\text{rust}} &= \Delta M_{\text{metal}} \cdot s_{\text{rust}} \cdot \text{MW}_{\text{rust}} / \text{MW}_{\text{metal}} \end{aligned} \quad (11.1.3-6)$$

where

ΔM_{gas} = mass of gas produced,
 ΔM_{metal} = mass metal corroded,
 $\Delta M_{\text{h}_2\text{o}}$ = mass water consumed,
 ΔM_{rust} = mass rust produced,
 $\text{MW}_{\text{material}}$ = molecular weight of a material.

Only the iron corrosion products were tracked in the 1994 PA, because we did not have estimates of the K_d 's for other corrosion products such as nickel or aluminum oxides.

11.1.4 Interface of GASSNF with BRAGFLO_T

As in the 1993 PA, the GASSNF submodel was included in BRAGFLO_T. BRAGFLO_T passes to a GASSNF routine the temperature, fracture saturation, and time step information. GASSNF passes back to BRAGFLO_T the gas and water production/consumption rates. Because the fracture saturation is, in theory, dependent on the gas and water production/consumption rates and these rates are dependent on the saturation, BRAGFLO_T may call GASSNF many times until a converged solution is reached. Once a converged solution is reached, BRAGFLO_T calls another GASSNF routine that updates the mass and breach state of each metal layer of each waste parcel. The coupling between the gas and water production/consumption rates and saturation were not expected to be nearly as tight as in the 1993 PA's salt disposal system, because water is not a controlling reactant when the repository is assumed to be oxid (as in the 1994 PA), and because the highly fractured host rock is quite permeable to gas flow.

An additional coupling that was not included into BRAGFLO_T and GASSNF in time for the 1994 PA calculations is the enthalpy of the corrosion reactions. The oxidation of metals such as iron, aluminum, and uranium, is highly exothermic and produces heat that could raise the temperature of the repository. However, because many phenomena are temperature dependent, including the corrosion rates, this feedback mechanism was left out of the 1994 PA. The possible effects of its absence in the 1994 PA are considered below.

When the corrosion rates are slow, as in the case of steels, the rate of energy input into the system from corrosion is negligible compared to the energy input from radioactive decay. Uranium metal, however, may have high corrosion rates if oxygen is plentiful, so the energy input rate may not be negligible at least locally. The energy from corrosion of all the N-Reactor fuels to schoepite ($\text{UO}_3 \cdot 2\text{H}_2\text{O}$) is 1.34×10^{10} kJ, which is 1/10 of the energy produced in the first year from decay and about 1/1000 of the total energy produced by year 1000. If all the uranium is exposed at the same time and corrodes at the fastest sampled corrosion rate, it will be consumed in 0.13 yr and release 3266 kW during that time. The slowest sampled corrosion rate would yield 32 kW for 13 yr. A single MPC of N-Reactor fuel would produce a median of 5.5 kW for 1.3 yr if all the cladding within the parcel failed at the same time, while a single LWT parcel would produce 827 W for 1.3 yr. This amount of energy has little effect at the repository scale, but might cause a significant temperature rise at the individual parcels.

If oxygen is readily available, the increase in temperature at the waste parcel will accelerate the corrosion rate, but it is not expected that the fuel would ignite because of the relatively low surface-area-to-mass ratio of these fuels. A more likely scenario is that as oxygen is consumed within the repository, and especially within the parcel, the uranium corrosion rate will be limited by the rate of oxygen inflow. The other possible reactant for oxidation of uranium is water. If the energy from uranium corrosion raises the local temperature above boiling, the liquid water will be driven off, and the corrosion will slow dramatically. Because the rates of water and oxygen flux are likely limiting factors, omission of the enthalpy effect is probably not significant. However, for the sake of completeness, this effect will be included in future calculations.

11.2 Source Term

The source term model is responsible for calculating the dissolution, sorption, radioactive buildup/decay and transport of radionuclides within and out of the WEPs. (Note the WEP includes both the waste parcel and any drift or borehole air gap or backfill.) These processes are very complicated in nature and many simplifications are necessary due to computational time constraints as well as lack of adequate models and data. The source term model used in the 1993 PA, CONCSNF, was written with simplifications that could be justified only for a saturated repository and the calculational mesh used in the 1993 PA. These features were not suitable to the unsaturated repository in the 1994 PA, so a new code, USATCONC, was written. This section describes the features and model simplifications of USATCONC. USATCONC was designed as a set of routines that may be called by a transport code such as NUTS or TOSPAC or may be called by the included driver routines in a stand-alone mode within the CAMCON system.

GASSNF, which provides USATCONC with the mass of rust at each location and time step and the times of breach of protective layers, was included within USATCONC for several reasons. The GASSNF routines are fast running and so it is nearly as fast to calculate the masses of rust within USATCONC as it would be to read them in from a transfer file. Also, because the repository fluid flow is not expected to be significantly affected by gas consumption, the inclusion of the GASSNF routines within USATCONC allows an analyst to vary the corrosion parameters without rerunning the flow calculations. Finally, the standalone version of USATCONC is more complete with GASSNF included, facilitating additional parametric studies.

11.2.1 Conceptual Model: Radioactive Decay/Buildup

With USATCONC, the user specifies which radionuclides and chains to include in the calculation in an input file. Of the 63 radionuclide isotopes listed in Appendix A, many are very short-lived and were included only because of their importance to the heat generation of the waste (see Chapter 4). Short-lived radionuclide isotopes do not accumulate in large amounts and are not regulated by 40 CFR 191. Removing unnecessary isotopes from the list was

required to prevent overwhelming the storage limits of the computers when USATCONC was run within NUTS. For the 1994 PA, 32 radionuclide isotopes were selected (see Table 11-2). The selection was based on the length of half-lives and whether the isotopes were present in significant amounts. The run time and storage limits for radionuclide isotopes that are modeled by the transport code are even greater than for the isotopes that are included within USATCONC. Consequently, of the 32 isotopes handled by USATCONC, only 12 were passed on to the transport codes NUTS and TOSPAC: ^{14}C , ^{79}Se , ^{99}Tc , ^{129}I , ^{231}Pa , ^{233}U , ^{234}U , ^{235}U , ^{236}U , ^{237}Np , ^{238}U and ^{239}Pu . These radionuclide isotopes were chosen based on the likelihood of their release from the regulated boundary within 100,000 yr as determined by the TSPA-1993, as well as other factors such as importance to criticality. Hence, the isotopes chosen for transport modeling are referred to here as the 12 "transported" isotopes.

USATCONC is responsible for radioactive decay/buildup of the 32 isotopes within the WEPs, while the transport codes, NUTS or TOSPAC, are responsible for radioactive decay/buildup of only the 12 transported isotopes once they are released from the WEPs. Because some of the "non-transported" isotopes such as ^{241}Am are parents of "transported" isotopes, it was also necessary for USATCONC to keep track of radioactive buildup/decay from the "non-transported" isotopes even after they are released from the WEPs. Accordingly, for each grid block all non-transported isotopes released from the WEPs are stored and decayed. At each time step, the amount of each "transported" isotope generated by decay of released "non-transported" isotopes is calculated and added to the release of that isotope. In this way, the error from not transporting all 32 isotopes is minimized. The effect is as if all non-transported isotopes have infinite K_d 's once released from the WEPs and thus they remain within the waste grid blocks.

11.2.2 Conceptual Model: Location of Radionuclides within the WEPs

USATCONC defines five locations within the waste emplacement packages where the isotopes may reside (Figure 11-3):

Location Description

- 1,2 matrix, up to two matrices
- 3 unbound solids within the parcel
- 4 dissolved within the pore fluid in the parcel
- 5 absorbed onto the rust from the corroded iron-containing WEP layers.

Isotopes are released at each location as follows:

- 1,2 **Matrices.** Initially, all radionuclide inventory resides in the matrix(es). Within spent fuel matrices, such as UO_2 , some separation of radionuclides from the bulk matrix into grain boundaries or the gap between the matrix and the cladding may have occurred. The fraction of each radionuclide that has migrated into these locations will be called the quick release fraction. At breach of the protective layers, the quick release fraction of the radionuclides is immediately moved into the unbound solids location, from which the radionuclides may dissolve up to their solubility limit. Other than the quick release fraction, the remaining radionuclides are assumed to be homogenous within the matrix. These radionuclides are assumed to be exposed to pore water (moved to the unbound solids location) at the same rate that the bulk matrix is dissolved or altered.
- 3 **Unbound Solids.** Once a radionuclide is no longer bound up in a matrix, it is free to equilibrate with the waste parcel pore fluids. The amount of fluid used in the equilibration calculation is the residual amount in the parcel plus the amount that passes through the parcel in the time step. When more than one isotope exists for an element (e.g., uranium), each isotope is dissolved in proportion to its relative abundance.
- 4 **Waste Parcel Pore Fluid.** The USATCONC routines model the equilibration of radionuclides between unbound solids, pore fluid and rust, as well as advection of pore fluid through the parcel and diffusion of radionuclides out of the parcel when a diffusion path is present. At present, colloids are not explicitly modeled.

Table 11-2. Isotopes Tracked by USATCONC and the Transport Codes

Transport Modeled?	Isotope	Daughter
x	^{14}C	
	^{59}Ni	
	^{63}Ni	
x	^{79}Se	
	^{90}Sr	
	^{93}Zr	
x	^{99}Tc	
	^{126}Sn	
x	^{129}I	
	^{135}Cs	
	^{137}Cs	
	^{147}Sm	
	^{151}Sm	
	^{226}Ra	
	^{229}Th	
	^{230}Th	^{226}Ra
x	^{231}Pa	
	^{232}U	
x	^{233}U	^{229}Th
x	^{234}U	^{230}Th
x	^{235}U	^{231}Pa
x	^{236}U	
x	^{238}U	^{234}U
x	^{237}Np	^{233}U
	^{238}Pu	^{234}U
x	^{239}Pu	^{235}U
	^{240}Pu	^{236}U
	^{241}Pu	^{241}Am
	^{242}Pu	^{238}U
	^{241}Am	^{237}Np
	$^{242\text{m}}\text{Am}$	^{238}Pu
	^{243}Am	^{239}Pu

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Figure 11-3. Locations of radionuclides in waste container. The source term submodel monitors these locations as protective layers are breached. The model must accommodate 9 sources of waste, each with a different radionuclide inventory, up to 8 nested layers that may react with water, and 10 different matrices, such as uranium dioxide and borosilicate glass.

- 5 Rust. Radionuclides are sorbed or desorbed in proportion to the concentration within the pore fluid using the standard linear proportionality constant K_d . (K_d is defined in Section 11.3.2.)

11.2.3 Mathematical/Computational Model

The inner algorithm of USATCONC calculates the radionuclide release for a single WEP type from a single container group in a single grid block. USATCONC loops over all container groups and WEP types within a grid block, summing the releases for calculation of the total grid block release rate which is passed on to the transport code. Release of radionuclides may be described as occurring in three steps: (1) change from a "bound" state to an "unbound state", (2) equilibration between waste parcel pore waters, unbound solids, and rust, and (3) transport out of the engineered barrier system.

Change from a "Bound" State to an "Unbound State". For radionuclides in the quick release fraction, this step occurs at breach of the clad layer; for the remaining radionuclides, this occurs as the matrix alters or dissolves. The alteration/dissolution process is modeled by two types of equations, rate equations as used in the GASSNF (Equations 11.1.3-1 to 11.1.3-4) for thermodynamically unstable matrices and a solubility-controlled dissolution equation for thermodynamically stable matrices. In an oxidic repository, the only stable matrix in the waste parcels that were modeled is the ceramic phase of the glass-ceramic waste form. Because diffusion within the ceramic mineral grains is very slow, radionuclides are primarily removed from their "bound" state as the minerals dissolve. Unfortunately, there are more than several ceramic minerals in the ceramic phase, and proper modeling would require both the concentration of radionuclides within each mineral type as well as the mineral solubilities. In addition, modeling the dissolution would require modeling the transport of the dissolved minerals out of the canister. Given additional time it would be possible to obtain reasonable estimates for the required parameters, but for the 1994 PA, the recommendation of the INEL researchers most familiar with this waste form was to use a simple rate three orders of magnitude slower than the alteration rate of borosilicate glass. The reaction rate equations (Equations 11.1.3-1 to 11.1.3-4)

are once again selected with the input parameter CORMOD. A CORMOD of 2 selects solubility-controlled dissolution. As in the GASSNF routines, corrosion rates are specified for both wet oxidic and humid oxidic conditions. For many of the matrices, the corrosion rate in humid conditions is zero, and for all matrices, the time dependence exponent, term C, was set to 1.

Equilibration between Waste Parcel Pore Waters, Unbound Solids, and Rust. This step determines the mass of each radionuclide that dissolves into the waste parcel pore waters from the unbound solids state and the amount that sorbs/desorbs onto the iron corrosion products of the waste parcel. Instantaneous, reversible equilibrium is assumed both for dissolution/precipitation as well as sorption. This assumption results in overestimated concentrations within the parcel when the flow rate is much faster than the radionuclide dissolution rate and when sorption is actually irreversible. The amount of an isotope calculated to dissolve depends upon its solubility, the amount of water in contact with the solids during the time step, and the sorptive capacity of the corrosion products. The volume of water in contact with the solids includes both a residual volume of water that is assumed to always be present once the parcel is breached and the volume of water that passes through the parcel during the time step. The residual volume was necessary to allow for release by diffusion when the flow rate is zero. The volume of pore water used in the equilibration is calculated as follows:

$$V = V_{\text{res}} + V_{\text{flow}} \quad (11.2.3-1)$$

and

$$V_{\text{flow}} = Q * CA_{\text{WP}} * 10^{\text{ECA}} * \Delta T \quad (11.2.3-2)$$

where

- V = the volume of water used for equilibration with unbound solids,
- V_{res} = the residual volume of water that remains within the parcel, this user input was set to 10 cc,
- V_{flow} = the volume of liquid that passes through the parcel in a time step,
- Q = the fracture and/or rock matrix grid volumetric flow rate divided by the appropriate grid fracture and/or matrix cross sectional area as passed from the transport code in m/s; for the WEPs with an intact air gap, only the fracture flow rate was used; for the WEPs with rubble, combined fracture plus matrix flow was used,
- CA = the physical cross section area of the waste parcel,
- ECA = the effective cross section area term (EFFCAREA, Section 11.4), a sampled input parameter used to model the uncertainty in the collection area for flow.

The flow of water through a breached container is a process that is not well understood and is likely to be quite stochastic in nature. Uncertainty in the size and location of the breach; travel path for the water; effects of fracture-matrix interaction on the flow into the parcel; and the effects of the presence or absence of rubble around the parcel on the flow may never be reduced. Some of this uncertainty was included in the term ECA, which was sampled from -0.5 to 0.5 in this calculation. Arguments may be made that the ECA term should reflect the range in hole sizes penetrating the parcel as well the possibility that fracture flow will follow the drift walls and ceiling and not drip onto the canister. Such considerations could lead to a decrease of many orders of magnitude in the low range for the sampled ECA and result in greatly reduced calculated flow volumes through the parcel. The range from TSPA-1993 was used for this parameter because no additional information was available. For WEPs with an intact air gap, the Q term included only the fracture flow, because there is no mechanism for matrix flow to enter the parcel with an intact air gap. For WEPs with rubble, we have conservatively used the total grid flow, both fracture and matrix, even though it is uncertain that the matrix-parcel interface would allow matrix flow to leave the matrix and enter the parcel. For a breached parcel, the following conditions were assumed: enough holes were present so that it was not necessary to model a delay time for filling the parcel, water was modeled as passing over the entire contents of the parcel before draining out, and the water was instantly saturated with all of the available radionuclides. A discussion of Q, the flow rate provided by the transport code, can be found in Chapters 12 and 13.

For the 1994 PA calculations, the solubility of a radionuclide is defined as the solubility of the element times the mole fraction of that isotope within that element. Because different isotopes of the same element have different half-lives, the mole fraction must be calculated at each time step, and care must be taken to include stable isotopes as well.

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When all isotopes are not included, as in the case of thorium in this calculation, the calculated solubility of the remaining isotopes are artificially high, which while not correct, is at least conservative.

The amount of each isotope that dissolves into the pore liquid is determined by the calculated parcel pore fluid volume, the isotope's solubility as defined above, and the sorption capacity of the corrosion products (rust) within the WEP as defined below, as long as enough of the isotope is available in the unbound solids location. When there is an excess of an isotope in the unbound solids state, the amount moved into the liquid and sorbed locations is determined by its solubility and K_d . When there is not an excess, all of the amount in the unbound solids is dissolved and proportioned between the liquid and sorbed locations according to the simple K_d model:

$$M_{\text{sorbed}} = K_d * C_{\text{liq}} * M_{\text{sorber}} \quad (11.2.3-3)$$

where M_{sorbed} is the mass sorbed, K_d is the simple linear partition coefficient, C_{liq} is the concentration of an isotope within the pore fluid, which is limited by its solubility, and the M_{sorber} is the mass sorbing material (in this case, rust) at each WEP is calculated by the GASSNF routines.

Transport out of the WEPs. This step is similar to, but not always the same as, the release from the engineered barrier system. 10 CFR 60 defines the engineered barrier system as including the WEPs as well as the underground workings. In the horizontal emplacement scheme, the WEPs are the waste parcels and the air gap or backfill surrounding them, which includes most of the underground workings, but in the vertical emplacement scheme, the WEPs include only the parcels and the air gap in the boreholes within which they are emplaced, but does not include the drifts.

The transport was modeled as two decoupled processes, advection and diffusion. Given the definition of V_{flow} , the volume of liquid passing through the parcel within a time step as discussed above, the mass advected within a time step, m_{adv} , is simply calculated as the product of V_{flow} and the concentration of the isotope within that water, C_{liq} .

$$M_{\text{adv}} = V_{\text{flow}} * C_{\text{liq}} \quad (11.2.3-4)$$

Diffusion is difficult to model because little is known about the nature of the diffusive pathway. The repository has been designed so that no diffusive pathways will exist; however, we can not rule out degradation of the drifts and/or boreholes. If the drift ceiling crumbles and piles debris up against the parcels, and if the corrosion process produces a hole where the debris is in contact with the parcel, then a diffusive pathway may be created. The size of the hole may range from a pinhole to the full surface area of the parcel. The nature of the debris is also unknown so the pathway from the hole to the host rock may be relatively straight or tortuous, and may have water saturation similar to the fracture or the matrix. Conca [1990] presents data and a convenient equation relating effective diffusion coefficient to the saturation of well-defined tuff gravels. The data show that as the gravel saturation falls, the effective tortuosity of the diffusion path may climb several orders of magnitude. Conca's equation however, applies only to the well-defined tuff gravels that he studied. Given the large uncertainties, we decided to model this process with a simple 1D diffusion equation and lump all uncertainty into one term, EDA:

$$M_{\text{diffused}} = D_{\text{mol}} * \text{EDA} * SA_{\text{WEP}} / l_{\text{airgap}} * (C_{\text{can}} - C_{\text{block}}) * \Delta T \quad (11.2.3-5)$$

where

M_{diffused}	=	moles diffused
D_{mol}	=	the molecular diffusion coefficient of the isotope in the water
EDA	=	a sampled parameter (see EFFDAREA, Section 11.4) to account for the uncertainty in the hole size and path tortuosity
SA_{WEP}	=	the surface area of the WEP
l_{airgap}	=	the shortest distance between the parcel and the host rock at emplacement
C_{can}	=	the concentration of an isotope within the canister
C_{block}	=	the concentration of an isotope within the grid block as passed from the transport code
ΔT	=	the time step size

Like the Q and ECA in advective releases, the EDA for diffusive releases is a crucial parameter that is not well known. The ranges chosen for ECA and EDA determine the calculated relative importance of advective and diffusive releases. Another simplification used in the modeling of diffusive transport is that the "potential diffusive release" is calculated from the concentration gradient at the start of the time step. No account is taken for the possible decrease in the concentration gradient during the time step. If the amount of an isotope present in the unbound solids, liquid and sorbed locations is greater than the calculated "potential diffusive release," the entire amount of "potential diffusive release" is moved from those locations to the released location prior to the equilibrium step. This simplification may cause an overestimation of the diffusive releases if the concentration within the grid block rises significantly in a time step.

Sorption on the rubble during diffusive transport is not modeled by USATCONC. Given the large uncertainties already described, this smaller effect has been conservatively left out.

Detailed Steps Performed Each Time Step. At each time step and for each type of waste parcel and each container group per grid block, USATCONC performs the following steps:

1. Calls the GASSNF routines. These routines update the amount of rust at each WEP and update the breach state of each layer of each WEP.
2. Calculates the maximum amount of each isotope that may diffuse from WEPs with bridged air gaps. C_{block} is assigned for each isotope as follows. For the transported isotopes, this value is passed from the transport code. For non-transported isotopes that are the same element as a transported element, this value is scaled from the transported isotope's concentration based on the isotope's relative abundance. For other isotopes, this value is conservatively set to zero. C_{can} is set to the concentration within the parcel at the last time step.
3. Updates the liquid volume for use in the equilibration step based on the time step's flow rate.
4. Calculates the radioactive buildup and decay of all isotopes in all locations and updates the isotope masses to the end of the time step. This step includes the calculation of the ingrowth of transported isotopes from non-transported isotopes in the released location.
5. Checks to see if any matrix within the parcel is exposed by the breach of the layers covering it. If no matrices are exposed, the model skips to the next parcel. If a matrix is exposed since the last time step, the quick release fraction of each isotope is moved from the matrix to the unbound solids location.
6. Recalculates the mass fraction of each isotope within each matrix and the relative abundance of each isotope for each element released from the matrix into the unbound solids, liquid, and backfill.
7. Calculates the amount of matrix that either is dissolved or altered within the time step.
8. Based on the mass of matrix altered in Step 7 and the mass fraction of each isotope in the matrix calculated in Step 6, moves the appropriate amount of each isotope from the matrix to the unbound solids location.
9. Equilibrates all isotopes among the unbound solids, pore fluids, and backfill using the solubilities and Kd's of the elements and the relative abundance of each isotope as calculated in Step 6. When the amount of an isotope is limited, the model conservatively removes the amount diffused first. The amount diffused is limited to the amount in the unbound solids location plus 10% of the amount in the liquid location.
10. Moves mass of each isotope dissolved in advecting pore fluids to "released" location.
11. Passes the total release of each radionuclide, due to advection, diffusion, and in-growth during the time step divided by the time step duration to the transport code.

For each grid block, the amounts released by all the WEPs and container groups are summed and passed on to the transport code. Mass balance calculations are also performed, and the summaries of the releases, and radionuclide locations, breach times for WEPS, etc. are output.

11.2.4 Summary of Modeling Assumptions

- The repository has been modeled as a uniform mix of the nine WEP types. In a real repository, it is most likely that there would be regions within the repository that have quite distinct distributions of the various WEP types.

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- The corrosion equation, Equation 11.1.3-1, has terms for an Arrhenius temperature dependence, a simulated step function for saturation dependence, a linear oxygen concentration dependence, and a time dependence. Terms for concentrations of corrosive species, and pH, were not included so variations in these variables were lumped into the pre-exponential term.
- Term D in Equation 11.1.3-1, the saturation-dependent corrosion term, is the only indicator of the wetness of the waste parcels. This term is determined by the saturation of the fracture as passed from the transport code when the grid block or the waste parcel is below the boiling point. Above the boiling point, a waste parcel is assumed to be in a humid environment. Unless separate temperature profiles are used, all waste parcels within a grid block experience the same fracture saturation and temperature even though it is known that the heat generation is not uniform across the waste parcel types.
- The radionuclide inventory in the matrix(es) of the waste form is assumed to be released congruently as the matrix alters except for the quick release fraction of each isotope, which is released instantly at the time of matrix exposure. Released radionuclides are moved to the unbound solids location from which they may dissolve up to their solubility limit.
- The temperature dependence of solubility is not directly modeled but is included in large solubility ranges.
- Matrix alteration occurs from one of two simplified mechanisms: solubility limited dissolution or constant rate alteration.
- The surface area of each matrix used in alteration rate calculations is set to the original outside area and not changed with time. When the surface area is uncertain, for example with fractured glass, the simple outside area is used and the uncertainty in the surface area is added to the uncertainty in the alteration rate.
- Sorption is modeled as reversible using a simple partition coefficient.
- Water entering a parcel is assumed to come to equilibrium saturation instantaneously.
- Filling of a parcel with its residual volume of water is assumed to be instantaneous.
- The fraction of WEPs with rubble bridging the air gap does not change with time.
- The only water contact modes for WEPs with intact air gaps are dripping and flooding. Condensation is ignored. Dripping and flooding are determined by the fracture saturation passed by the transport code. WEPs with rubble may contact fracture water directly.
- Diffusion is modeled with a simple 1-D equation with all the uncertainty in the diffusion area and path tortuosity lumped into one parameter.
- The volume of water used in advective releases is determined by the fracture flow rate only for WEPS with intact air gaps but total flow rate for WEPs with rubble. These volumetric flow rates are divided by their grid cross section area and then multiplied by the WEP effective cross section area to obtain a waste parcel flow rate. All the uncertainty in the water contact mode is bundled into the effective WEP cross section area term.

11.3 Modeling Parameters for Waste Parcel Corrosion and Source Term Models

The modeling parameters used by GASSNF and USATCONC for the waste parcels, elements, and radionuclides, respectively are summarized in tables in Section 11.4. The parameters for the 1994 PA were of necessity chosen in a very short period of time. An exhaustive review of the literature was not possible; instead, recent literature, review articles, and personal communications with various experts were used as guidance in making educated guesses.

11.3.1 Modeling Parameters for Waste Parcels

General Waste Package Parameters:

EFFCAREA - Effective Collection Area Term

0, -0.5 to +0.5 uniform distribution

As indicated in TSPA-1993, there is great uncertainty in the effective collection area for dripping onto the canisters. Because no further information has become available since the publication of TSPA-1993, its range was used

for this parameter, i.e., a half order of magnitude above and below the physical cross sectional area of the canister. Using Equation 11.2.3-2, ECA is set to range from -0.5 to 0.5.

EFFDAREA - Effective Diffusion Area Term

1×10^{-6} to 1, loguniform distribution

EFFDAREA is the term (EDA) in Equation 11.2.3-6 that accounts for the uncertainty in the hole size and tortuosity of a diffusive path from the altering matrix to the host rock. An EFFDAREA of 1.0 is used to model a waste parcel with a diffusional area that equals the surface area of the parcel, with a rubble tortuosity of 1. Given overpack surface areas of tens of square meters, a pinhole 1 mm in diameter is 7 orders of magnitude smaller than the overpack surface area. Because Incoloy is expected to fail by pit corrosion, it is expected that the area for diffusion may well be many orders of magnitude smaller than the parcel surface area for a very long time. Even if the canister offered no resistance to diffusion, the effective diffusional area could still be quite small because of poor contact with the rubble. Besides rubble, another mechanism for development of a diffusional pathway is corrosion and collapse of the supporting railroad car or stand. In this case, up to one quarter of the parcel surface area could be directly connected to the floor of the repository through a mass of porous corrosion products.

In addition to the 7 orders of magnitude of uncertainty in the effective diffusion area, the uncertainty in the tortuosity of the diffusional pathway may be many orders of magnitude. Conca (1990) reports the effect of water saturation on the effective diffusion coefficient. The measured effective diffusion coefficients ranged from below detection limits (1×10^{-11} cm²/s) when the gravel was below residual saturation to 1×10^{-5} cm²/s when the gravel had a 40% volumetric water content. With volumetric water contents of 4 to 9% the measured effective diffusion coefficients ranged from 2×10^{-9} to 2×10^{-7} cm²/s. Because the effective diffusion coefficients were found to depend on surface water content only and because the surface water content was a function of gravel grain size, these results are applicable only to the gravel sizes measured. Given the large uncertainties in both diffusion area and path length, an even six orders of magnitude was chosen for this parameter.

EBFRAC - Juvenile Failure Fraction

0.005, 0 to 0.01 uniform distribution

The juvenile failure fraction is defined as the fraction of waste parcels within the repository that have a breached outer layer at time zero. This breach may be due to manufacturing defects, damage that occurs during transportation and emplacement, or any other reason. SKB (1992a) used 1×10^{-3} . TSPA-1993 used juvenile failure fractions of 0.1 to 0.5% for the canisters without the carbon steel overpack and 0.05 to 0.25% for the canisters with the carbon steel overpack. In the 1993 PA, a decision was made to be more conservative and used a high of 1%, but also extend the low range to 0. Due to lack of time to further investigate this parameter, this range was also used in the 1994 PA.

BACFRC - Fraction of Parcels with Rubble

0.5, 0 to 1 uniform distribution

The fraction BACFRC is unknown and expected to be a function of time. As in TSPA-1993, a uniform distribution between the theoretical extremes, 0 and 1, was used.

TS and S99 - Saturation-Dependent Corrosion Terms for Equation 11.1.3-2

TS _a	.04
TS _b	0
S99 _a	.08
S99 _b	.08

TS_a is the threshold fracture saturation below which wet corrosion does not take place for waste parcels with an intact air gap. This parameter was set to the residual saturation of the fracture that was used in the simulations, 0.04. If condensation does not occur, then dripping is the only mechanism for water contact and dripping cannot occur unless the fracture is above residual saturation.

TS_b is the threshold fracture saturation below which wet corrosion does not take place for waste parcels with the air gap bridged by rubble or backfill. This was conservatively set to the theoretical minimum, 0.

S_{99a} and S_{99b} are the fracture saturations where wet corrosion is assumed to proceed at 99% of the fully flooded rate, a for airgap, b for bridged airgap. It is not known at present how corrosion rates will vary with fracture saturation or flow. Accordingly, not only these parameters but also the saturation-dependent Equation 11.1.3-2 are only guesses. The terms S_{99a} and S_{99b} were set to twice the fracture residual saturation. At twice the residual fracture saturation, there may be enough flow to keep the surface of the containers wet 99% of the time.

Material-Specific Waste Package Parameters:

All sampled corrosion parameters used loguniform distributions. For sampled parameters, the values are presented as median, low, and high. A CORMOD of zero indicates the use of the corrosion equation, Equation 11.1.3-1. A CORMOD of 1 was used for materials where the surface area was hard to determine. For these materials, corrosion term A is given in units of 1/s and the mass of the layer is used in Equation 11.1.3-3 instead of the surface area. A CORMOD of 2 indicates that alteration is solubility limited and a CORMOD of 3 indicates the use of Equation 11.1.3-4.

<i>Aluminum</i>		
CORMOD		0
COR_A_WO		$2 \times 10^8 \text{ kg/m}^2\text{s}$
COR_B_WO		0 K
COR_C_WO		1
FRCPENWO		0.5
COR_A_HO		$2.3 \times 10^{18} \text{ kg/m}^2\text{s}$
COR_B_HO		22000 K
COR_C_HO		.5
FRCPENHO		.5

Wet-Oxic Corrosion. The corrosion rate of aluminum in sea water (LaQue, 1975) ranged from 2×10^{-8} to $4 \times 10^{-7} \text{ kg/m}^2\text{s}$, while Godard (1960) reports penetration rates equivalent to 3×10^{-8} to $1.5 \times 10^{-5} \text{ kg/m}^2\text{s}$ in 17 Canadian fresh waters. The slowest fresh water rate would cause penetration of the ATR's 15-mil-thick aluminum cladding in one year, which is very short compared to the model time steps. Godard (1960) reports the importance of pH, total hardness, chloride, oxygen, copper, and water flow rate on the corrosion resistance of aluminum. In stagnant waters, he reports that pitting is responsible for the penetration of aluminum and that the pit penetration depth is the cube root of time. Godard also reports a temperature dependence of pit corrosion that has a sharp peak at 40°C. Given the very short service time reported by Godard, the use of time and temperature corrosion terms was deemed unnecessary and a single value of $2 \times 10^{-8} \text{ kg/m}^2\text{s}$ was chosen. Use of a FRCPENWO of 0.5 results in a penetration rate of $4 \times 10^{-8} \text{ kg/m}^2\text{s}$.

Humid-Oxic Corrosion. There are very few studies of the corrosion rate of aluminum at temperatures above 30°C. The Corrosion Data Survey (Hamner, ed., 1974), however, reports that above 100°C in air, aluminum corrodes at greater than 50 mils/yr. Given the thickness of the aluminum clad in the ATR fuel elements, this rate results in total corrosion of the clad in 0.33 yr, which is very small relative to the model time steps. If the equivalent corrosion rate of $1 \times 10^{-7} \text{ kg/m}^2\text{s}$ without any temperature dependence was used, the code would always pick the humid oxic rate over the wet oxic rate, which is incorrect. To prevent this, a rate of 1×10^{-8} at 90°C and 1×10^{-7} at 100°C was used to get an Arrhenius pre-exponential term of $2.36 \times 10^{18} \text{ kg/m}^2\text{s}$ and a temperature term of 22,000 K. These terms result in the use of the wet oxic rate of $2 \times 10^{-8} \text{ kg/m}^2\text{s}$ below boiling and a much faster rate when the temperature is above boiling. A FRCPENHO of 0.5 was used to be consistent with the FRCPENWO of 0.5.

Calcine

CORMOD 1

COR_A_WO 4×10^{-7} /s

COR_B_WO 0

COR_C_WO 1

COR_A_HO 0

COR_B_HO 0

COR_C_HO 1

Leach experiments show nearly quantitative removal of non-solubility limited elements in 28 days (see Appendix A). Assuming a constant rate of dissolution/alteration in the 28 days results in a fractional release rate of 4×10^{-7} /s. We have assumed that without water, the leach rate is zero.

Carbon Steel ASTM Grade 516

CORMOD 0

COR_A_WO 9.49×10^{-5} , 3×10^{-5} to 3×10^{-4} kg/m²s

COR_B_WO 2530 K

COR_C_WO 1

FRCPENWO .1

COR_A_HO 4.73 kg/m²s

COR_B_HO 6870 K

COR_C_HO 0.33

FRCPENHO 0.9

Wet-Oxic Corrosion. The INTERA performance assessment (Andrews et al., 1994) used two experts, David Stahl and Alan Lamont, to provide corrosion data for carbon steel. Stahl provided a time dependent corrosion equation:

$$P = 2,525,000 t(y)^{0.47} \times 10^{2850/T}$$

where

P = penetration in microns,

t = time (yr)

T = temperature (K)

and a pitting factor of 4 (pitting penetration is 4 times faster than general corrosion penetration). The equation and the pitting factor were obtained from a Westinghouse report that studied the temperature dependence of the corrosion rate of cast steel and iron in brine and seawater as well as the time dependent corrosion and pitting of carbon steel in Gatun Lake. The Westinghouse report estimated the error band for its equation to be about $\pm 25\%$. Stahl reports that the time exponent of 0.47 is further supported by some studies of corrosion in river waters that yield time exponents from 0.5 to 0.8 and the temperature term of 2850 K is similar to the term of 2300 K derived from data by S. Pednekar. The pitting factor from the Gatun Lake data ranged from 2.6 to 3.4, which Westinghouse rounded up to 4 for conservatism. Stahl also reported D. McCright's pitting factors of 0.9 to 3.2.

Lamont provided a time invariant corrosion rate with a parabolic temperature dependence with a maximum rate of 0.38 mm/yr at 80°C, a 20°C rate of 0.12 mm/yr. and a 100°C rate of 0.2 mm/yr.

Soo, Ed. (1984) reviewed the DOE Waste Package Program and summarized the work of Kirby (1979) and Uhlig (1971) on the pH, temperature, and oxygen concentration effects on the corrosion rate of carbon steel. From the ranges of corrosion rates presented from Kirby's work, the Arrhenius corrosion rate terms of 2530 K and 3×10^{-5} to

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Figure 11-4. Corrosion rates.

$3 \times 10^{-4} \text{ kg/m}^2\text{s}$ were obtained and used in this analysis. Figure 11-4 shows the temperature dependence of the used Lamont, and Stahl corrosion rates. The Stahl corrosion rates are time dependent and are plotted for several time spans. Note that the corrosion rates used in the calculations are almost identical to the Stahl corrosion rates at 20 yr; the Lamont rates are similar. The decrease in corrosion rates above 80°C in the Lamont rate is due to decreased O_2 solubility in water at high temperatures in an open system. In a closed system, the rate would continue to increase with temperature. Because the proper modeling of O_2 transport and consumption has been left for future work, the Lamont equation was not used this year. After consultation with R. Westerman (1994), the decision was made to not use the Stahl equation. Westerman argued that time-dependent corrosion rates are difficult to defend over a 10,000-yr period. In practice, corrosion often undergoes a parabolic decrease in rate at early times, but then reaches a long term linear rate. Westerman suggested using the longest time of the experiments and use the linear rate to that time. This method may overestimate the corrosion rate at late times, but it is defensibly conservative. Because the Gatun Lake time-dependent results were obtained from a 16-yr study, and because the Stahl corrosion rates at 20 yr agree so well with the parameters calculated from Kirby's data, using these parameters derived from Kirby's data appeared to be justified.

Humid-Oxic Corrosion. Oxic corrosion of carbon steel in a humid environment is very slow except at very high temperatures. Very little corrosion is expected as the result of humid corrosion because canister temperatures are not anticipated to rise much above 200°C . The parameters from Stahl (1993) are included for completeness sake.

Ceramic - The Ceramic or Mineral Phases in the Glass-Ceramic Waste Form

CORMOD	0
COR_A_WO	1×10^{-14} , 1×10^{-17} to $1 \times 10^{-11} \text{ kg/m}^2\text{s}$
COR_B_WO	0
COR_C_WO	1
COR_A_HO	0
COR_B_HO	0
COR_C_HO	1

The ceramic or mineral phases of the glass-ceramic waste form are expected to be stable within the proposed repository. Their dissolution rate should be solubility and not rate limited. Because there are several ceramic minerals, proper modeling requires input of the solubility of each mineral, as well as the fraction of each isotope within each mineral. During dissolution, modeling of the transport of each of the dissolved mineral species from the canister is also required. Given sufficient time it would be possible to obtain reasonable estimates for the required parameters, but for the 1994 PA, the recommendation of the INEL researchers most familiar with this waste form was to use a simple rate three orders of magnitude slower than the alteration rate of borosilicate glass.

Glass - DOE Borosilicate Glass or Glass Phase in the Glass-Ceramic Waste Form

CORMOD	0
COR_A_WO	1×10^{-10} , 1×10^{-12} to 1×10^{-8} kg/m ² s
COR_B_WO	0
COR_C_WO	1
COR_A_HO	0
COR_B_HO	0
COR_C_HO	1

Many studies of glass dissolution have been performed, and many glass dissolution models have been proposed in the last 20 years. These models and experiments, however, have focused mainly on the short term of glass dissolution in distilled water. Dissolution into unsaturated tuff groundwater is expected to proceed much slower due to the high dissolved silica content of these waters. Long-term dissolution rates such as those reported by Strachan et al. (1990) are more likely to be applicable to the long term performance of glass in a silica rich repository. Unlike the short term rates, the temperature and pH dependence of these long term rates are not well defined.

Strachan et al. (1990) report final dissolution rates for PNL 76-78, SRL-165, and EMS-11 glasses (Figure 3.1 of their report) as 0.08, 0.02, and 0.002 g/m²d, respectively. The final dissolution rate is defined as the rate when the solution is saturated with respect to SiO₂. These rates correspond to a range of about 2×10^{-10} to 2×10^{-11} kg/m²s. Interaction of the silica rich waters with a carbon steel overpack may reduce the silica concentration of the water and increase the glass dissolution rate toward the rate measured in short term experiments, 1×10^{-8} kg/m²s (McVay and Buckwalter, 1983). In contrast to these relatively fast alteration rates, Crovisier et al. (1989) report alteration rates of basaltic glasses (considered by many to be good natural analogs to high-level waste glass) of 2×10^{-16} to 1×10^{-12} kg/m²s.

There is also uncertainty in the glass surface area. In the calculation, the monolithic surface area was used. Because this is the low end of some actual range, two orders of magnitude were added to the upper limit of the alteration rate to account for glass fracturing that may increase the surface area.

Graphite

CORMOD	0
COR_A_WO	4.79×10^1 kg/m ² s
COR_B_WO	17,200 K
COR_C_WO	1
FRCPENWO	0
COR_A_HO	4.79×10^1 kg/m ² s
COR_B_HO	17,200 K
COR_C_HO	1
FRCPENHO	0

Lotts et al. (1992) report an extrapolated oxidation rate of graphite at 100°C as $4. \times 10^{-20}$ g/cm²s for 0.1 atm O₂ pressure and 1.05×10^{-17} g/cm² at 150°C. While extrapolation from data collected above 400°C to such low temperatures is suspect, the rate at low temperatures is too slow for direct measurement; therefore two data points for an

11. Parcel Corrosion and Source Term Models

Arrhenius fit were used to obtain the corrosion terms reported above. A decision was made to ignore the possible effect of catalysis due to salts present even though catalysis by calcium potassium oxides has been reported (Pereira et al., 1992) for the gasification of graphite at high temperatures. These experiments showed that the temperature necessary for commercially acceptable rates of gasification was lowered from 1400 K to 800 K. It is not clear that the catalysis mechanism would be the same at below 100°C.

The perforation fraction was set to zero to echo our assumption that the time for water to soak through the graphite is very small compared to the time steps of the calculation.

Incoloy 825

CORMOD	0
COR_A_WO	5.6×10^{14} , 5.6×10^{13} to 5.6×10^{15} kg/m ² s
COR_B_WO	19,600 K
COR_C_WO	1
FRCPENWO	0.03
COR_A_HO	4.56×10^{-3} kg/m ² s
COR_B_HO	13,200 K
COR_C_HO	1
FRCPENHO	0.03

Wet Oxid. From TSPA-1993, Table 13-5, the 95th percentile was used for the deepest pits at 70°C and 100°C. An Arrhenius fit of these values gives a temperature term of 19,600 K and a median pre-exponential term of 1.87×10^{16} kg/m²s for the pit penetration rate. Comparison of Table 13-5 to Van Konynenburg et al. (1993) shows agreement between the median mean growth rate of pits of 1×10^{-3} mm/yr. Van Konynenburg et al. also report a generalized corrosion rate of 3×10^{-5} mm/yr which is 0.03 times the localized corrosion rate. Because localized corrosion is most important for the penetration of Incoloy Alloy 825, the activation energy for the Incoloy Alloy 825 was used in the generalized corrosion equation (see Equation 11.1.3-5). The pre-exponential term for general corrosion is then 0.03 times the pre-exponential term for localized corrosion, 5.6×10^{14} kg/m²s. The use of a FRCPENWO of 0.03 with these terms will result in a median penetration rate consistent with Table 13-5. The high and low ranges for the pre-exponential term were similarly obtained from the data in Table 13-5.

Humid Oxid. TSPA-1993 quotes dry corrosion rates for Incoloy at 25°C and 253°C. An Arrhenius fit to these points yields the terms shown. Note that at 100°C, the humid rate is more than 9 orders of magnitude slower than the wet rate and it does not reach the 100°C wet rate until 727°C. Without liquid water, the galvanic cell that is required for pitting corrosion cannot occur, thus pitting corrosion can not occur in a humid environment, but stress corrosion crack is still possible.

Metal Carbide - UC₂ and ThC₂ Fuel Meat

CORMOD	1
COR_A_WO	1×10^{-9} /s
COR_B_WO	0
COR_C_WO	1
FRCPENWO	0
COR_A_HO	1×10^{-9} /s
COR_B_HO	0
COR_C_HO	1
FRCPENHO	0

From Appendix A (Volume 3 of this report), an estimate can be made that it will take 17 yr to consume all the available carbides using a reasonable rate derived from a mechanism of a cyclic thermal suction of water into the cracked particles. Total consumption in 17 yr is equivalent to 1.86×10^{-9} removed per second. Seventeen years is

about equal to the smallest times steps used in the simulation, and so this rate is effectively instantaneous and sampling over a range would not be necessary. Because carbides are quite reactive in humid air (Wilkinson, 1962), and the graphite block and cracked particles impose transport resistance to incoming oxygen or water vapor, the same rate was used in a humid environment as in a wet one. The FRCPENs are irrelevant because the carbide is the innermost layer.

Stainless Steel 304L and Borated Stainless Steel 304L

CORMOD	0
COR_A_WO	1×10^{-13} , 1×10^{-16} to 1×10^{-10} kg/m ² s
COR_B_WO	0
COR_C_WO	1
FRCPENWO	0
COR_A_HO	1×10^{-13} , 1×10^{-16} to 1×10^{-10} kg/m ² s
COR_B_HO	0
COR_C_HO	1
FRCPENHO	0

Wet Oxid. After discussions with Richard Westerman (1994) in which he stated that wet stainless steel is susceptible to stress corrosion cracking above 60°C, the FRCPEN of stainless steel was set to zero, assuming the stainless steel will breach immediately. Given this assumption, the significance of corrosion becomes two-fold: the production of rust (not very important) and the release of boron from the borated steels (extremely important to criticality issues). At present, no studies were found that measured the release rate of boron from borated stainless steels in repository-type conditions. After discussion with Rudy Bucheit of Sandia National Laboratories (1994), a researcher who studied borated steels for Carpenter Technologies, an attempt was made to bracket the possible release rate.

Studies show boron is not very soluble in stainless steel and migrates to the grain boundaries along with chromium forming chromium borides. Metal borides in general (Cotton and Wilkinson, 1972) are very hard, refractory, usually chemically inert, and have very unusual properties due to the strong covalent metal-boron bond. The boron may exist as isolated boron atoms within the metal structure, as boron chains, as close packed boron layers or as a three dimensional network. Because the M-B bond is so strong, it is likely that the bulk stainless steel will corrode faster than the borides, which will remain as small unreacted particles within the corrosion products. In order to bracket the possible behavior of the borated steels, the release of boron was modeled as if it were congruent with the general corrosion of the steel, but the stainless steel corrosion rate was varied over a large range. Van Konynenburg et al. (1993) report a generalized corrosion rate of 0.1 micron/yr for stainless steel 304L, which is equivalent of 2.54×10^{-11} kg/m²s. This number may come from McCright et al. (1987), which reports about 0.1 microns/yr generalized corrosion rate at 100°C and is probably near the high end of possible corrosion rates. This value was rounded up to 1×10^{-10} as our high range.

The boron release rate predicted by use of this high range value could occur only if the chromium oxide protective coating on the stainless steel does not become more protective as it thickens, if the M-B bond is as weak or weaker than the Fe-Fe bond, and if the conditions within the repository remain as hostile as the experimental conditions for a period of time. For the low range, a time-dependent equation given by Jones and Greene (1966) was used, which assumes that the protective quality of the chromium oxide coating continues to increase as the reaction proceeds. The total corrosion predicted by this equation to occur in 10,000 yr was calculated. When this number is divided by 10,000 yr, a very low uniform corrosion rate of 3.5×10^{-16} kg/m²s is obtained. Rounding to 1×10^{-16} for the low range, the parameter's range is 6 orders of magnitude. Future studies on the release rate of boron from borated steels and the long-term behavior of the oxide coating on stainless steels should help to narrow this range considerably. The high range is anticipated to be conservative but enough information to estimate the true value is not available.

Humid Oxid. There is as much uncertainty in the humid-oxidic corrosion rate as the wet-oxidic corrosion rate for stainless steel 304L. McCright et al. (1987) report a generalized corrosion rate at 150°C of 0.075 microns/yr, which

is slower than the 0.1 micron/yr rate at 100°C. Given the large uncertainty, we chose to use the same range for humid-oxic corrosion as wet-oxic corrosion.

TRISO Coating for Metal Carbide Fuel

CORMOD	1
COR_A_WO	3×10^{-12} /s
COR_B_WO	0
COR_C_WO	1
FRCPENWO	1
COR_A_HO	3×10^{-12} /s
COR_B_HO	0
COR_C_HO	1
FRCPENHO	1

Lotts et al. (1992) report that only unknown mechanisms will breach unfailed particles within a repository. Rate term "A"s of about 1/10,000 yr (3×10^{-2} /s) and FRCPENs of 1 were used to reflect the assumption that TRISO will not fail in 10,000 yr.

Uranium

CORMOD	0
COR_A_WO	9.4×10^3 kg/m ² s
COR_B_WO	7970 K
COR_C_WO	1
COR_A_HO	1.35×10^2 kg/m ² s
COR_B_HO	7240 K
COR_C_HO	1

Wet Oxic. Wilkinson (1962) quotes rates for uranium corrosion at different temperatures with water saturated with different gasses. The corrosion rate at 50°C in water saturated with hydrogen (1.83×10^{-7} kg/m²s) is faster than the rate with water saturated with oxygen or air. At 90°C, the rates in oxygen and hydrogen saturated water are equal (2.78×10^{-6} kg/m²s). Because water within the canister may well be depleted of oxygen and saturated with hydrogen, we chose to use the faster hydrogen saturated rate. An Arrhenius fit to the reported values gives the corrosion terms as shown.

Humid Oxic. Wilkinson (1962) reviews the behavior of uranium in humid environments. Ea/R's range from 5000 K to 10,000 K, depending on the conditions of the experiments and corrosion products which range from protective (for example UO and UO₂) to non-protective (for example U₃O₈ and UH₃). The entries on Table 7 of Wilkinson (1962, p. 802) for 138°C and 200°C were used for an Arrhenius fit. These result in a pre-exponential term of 1.35×10^2 kg/m²s and a temperature term of 7240 K.

There has been some concern over the large enthalpy of reaction between uranium and water or oxygen. As the reaction progresses, the temperature of the metal increases unless the heat of reaction can be quickly conducted away. When the surface area to volume ratio of uranium is very high, the heat of reaction cannot be adequately conducted away and the uranium will ignite; however the ignition temperature for massive uranium in air is greater than 700°C. Also, the inflow of oxygen or water in the canister will be limited, which will decrease the chance of ignition. It is expected that under repository conditions, the uranium will undergo a moderate rise in temperature to a steady state, which will be determined by the uranium surface area, the thermal contact of the uranium with other canister metals, and the rate of inflow of oxygen and/or water. The corrosion rates modeled in the 1994 PA have ignored this local

heating effect, and thus may be low. However, the rates are fast enough for the uranium within a fuel rod to be consumed in less than a time step, so this effect may not affect the PA results.

Uranium-Aluminum Alloy Fuel

CORMOD	0
COR_A_WO	$2 \times 10^{-6} \text{ kg/m}^2\text{s}$
COR_B_WO	0 K
COR_C_WO	1
COR_A_HO	$1.35 \times 10^2 \text{ kg/m}^2\text{s}$
COR_B_HO	7240 K
COR_C_HO	1

Wet Oxid. Vinjamuri and Hobbins (1983) report erosion of UAl_x through a pinhole in the aluminum clad at ATR primary coolant conditions (2.45 MPa light water cooling). The pinhole was postulated to have formed at a hot spot estimated to be about 500°C. From the surface area of the resulting circular eroded area and the observed mass lost, the corrosion rate must have been greater than $2 \times 10^{-6} \text{ kg/m}^2\text{s}$ at the flow rates of 1.22 m/s. Wilkinson (1962) reports corrosion rates of uranium-aluminum alloys with 16% to 45% by weight uranium of $1.32 \text{ mg/cm}^2\text{hr}$ ($3.6 \times 10^{-6} \text{ kg/m}^2\text{s}$) in groundwater with 1 ppm Cl. With such rapid corrosion rates, it is necessary to obtain the rate only to within 2 orders of magnitude.

Humid Oxid. No data were found for the humid-oxid corrosion of UAl_x ; however, the corrosion terms for humid oxid corrosion of uranium metal yield a rate of $5 \times 10^{-7} \text{ kg/m}^2\text{s}$ at 100°C which is similar to the prediction of corrosion rates of greater than 1×10^{-7} for aluminum at that temperature. Because the UAl_x corrodes faster than the aluminum clad in ATR primary coolant environment, it is not unreasonable to use the uranium humid-oxid corrosion rate terms for UAl_x .

Uranium Dioxide Fuel

CORMOD	0
COR_A_WO	4.43×10^{-6} , 1.4×10^{-7} to $1.4 \times 10^{-4} \text{ kg/m}^2\text{s}$
COR_B_WO	3610 K
COR_C_WO	1
COR_A_HO	$1.72 \times 10^{-4} \text{ kg/m}^2\text{s}$
COR_B_HO	5989 K
COR_C_HO	1

Wet Oxid. Gray et al. (1992) examined the effect of temperature, pH, and carbonate concentration on the alteration rate of light water reactor (LWR) spent fuel at 0.2 atm O_2 partial pressure (air). The reported activation energy of 30 kJ/mole converts to 3610 K for the b corrosion rate term. Examination of the data in Table 3 in Gray et al.'s report shows a mean corrosion rate term "a" of $4.43 \times 10^{-6} \text{ kg/m}^2\text{s}$, with a range of about one half an order of magnitude. The high range was increased one order of magnitude to compensate for the use of the nominal surface area instead of the grain surface area. The low range was also decreased by an order of magnitude to account for possible saturation and depleted oxygen effects.

Humid Oxid. TSPA-1993 reports that humid oxid corrosion would take 100 yr to alter all the UO_2 at 250°C and 10,000 yr at 100°C. Using the mass and surface area for the UO_2 matrix within WP105, an Arrhenius fit to these estimates yields the corrosion terms reported above.

Zircaloy Cladding

CORMOD	0
COR_A_WO	$1 \times 10^{-12} \text{ kg/m}^2\text{s}$

11. Parcel Corrosion and Source Term Models

COR_B_WO	0 K
COR_C_WO	1
COR_A_HO	$6 \times 10^{-2} \text{ kg/m}^2\text{s}$
COR_B_HO	11173 K
COR_C_HO	1

Wet Oxid. Garisto and Garisto (1991) report a uniform corrosion rate for Zircaloy-4 of less than $1 \times 10^{-8} \text{ m/yr}$ or less than $2 \times 10^{-12} \text{ kg/m}^2\text{s}$. We rounded this down to 1×10^{-12} .

Humid Oxid. Garzarolli (1980) reports Arrhenius fits to data by several authors. The terms reported above are derived from the reported terms of Dalgaard.

Specific Parameters per Waste Parcel:

WP101, 201

ECFF 0.045, 0.037 to 0.053 uniform distribution

The fraction of damaged Fort St. Vrain and Peach Bottom fuel particles was estimated for 1993 PA. In the 1993 PA, a tail of 10% probability was given that the undamaged particles would breach in 10,000 yr. In the 1994 PA, the corrosion rate of TRISO was used to model this phenomenon so a uniform distribution from the calculated low to high was used.

WP102,202

ECFF 0.33, 0.16 to 0.5 uniform distribution

Pintner (1995) reported from visual inspection of the tops of the N-Reactor fuel rods that 9.6% of the inner rods have failed and 9.6% show signs of changes that may result in failure. The outer rods show more damage, with 19% failed and 10% with changes. The mass ratio of outer to inner rods is about 2.1. To obtain the low range, the weighted average of the observed failed rods, 16%, was used. Pinter estimated that the most probable failure rate would be obtained by assuming that half of the "changed" rods would fail, the bottoms of the rods would show the same failure rates as the tops, and the tops and bottoms were not correlated. These assumptions result in $14.4\% + (14.4\% \times 0.856) = 27\%$ failed inner rods and $24\% + (24\% \times 0.76) = 42\%$ failed outer rods. The resulting weighted average yields 37% failure rate. The high range was obtained by assuming that all of the rods showing changes would fail, the bottoms of the rods would show the same failure rates as the tops, and the tops and bottoms were not correlated. These assumptions result in $29\% + (29\% \times 0.71) = 50\%$ failure of the outer rods failed. We neglected to do the weighted average with the inner rods, which would have produced a maximum of 45%. The additional 5% may be justified by the argument that some of the damage may not be visible even as changes in the rods' appearance. A uniform distribution from 0.16 to 0.5 results in a median value of 0.33, which was felt to be close enough to 0.37 given the nature of our calculations.

QRF_M1C 0.02

The quick release fraction of 0.02 for ^{14}C on the surface of the Zircaloy clad was chosen after the value reported in TSPA-1993.

WP103,203,105,205

ECFF 1×10^{-2} , 1×10^{-3} to 1×10^{-1}

QRF_M1C	0.02
QRF_M2C	0.125, 0.01 to 0.25, uniform
QRF_M2Cs	0.081, 0.057 to 0.104, normal
QRF_M2I	0.081, 0.057 to 0.104, normal
QRF_M2Tc	0.06, 0.0367 to 0.0833, normal

McCoy and Doering (1994) report leaking commercial fuel rod fractions of 0.02% to 1% while Quinn and Thomas (1994) report that 4% of the total fuel inventory has known damage. Manaktala et al. (1994) report an assumed fraction of 0.01 to 0.02% breached rods, but also noted earlier fuel cores with as many as 33% failed rods. Using these failure rates for commercial fuel as a guide, a range of 0.1 to 10% early clad failure was used for our Shippingport and PWR waste parcels.

Garisto and Garisto (1991) give the distributions shown above for the fraction of C, Cs, I, and Tc, which have migrated into the gap or UO_2 grain boundary in commercial fuels.

WP104,204

ECFF 0

A good estimate of the fraction of ATR fuel with damaged aluminum clad was not obtained in time for this year's PA; however, given the high corrosion rate of aluminum, the exposure of fuel with damaged and undamaged clads probably occurs within the same time step.

WP106,107,108,109,110,111,206,207,208,209,210,211

ECFF 0

These reprocessed wastes have no highly protective "clad" analogous to Zircaloy or TRISO.

11.3.2 Element Parameters: Sorption and Solubility

The sorption and solubility of radionuclides affect their mobilization and transport from within waste parcels and along potential pathways away from the repository. Solubility and sorption are functions of the groundwater chemistry and temperature, which vary both in time and space. Some major geochemical variables include pH, Eh (SiO_4^{2-} , HCO_3^-), and temperature. Because of the uncertainty in the evolution of water chemistry and temperature both inside and outside the waste parcels, Sandia used an expert panel to obtain probability distribution functions for sorption and solubility parameters for TSPA-1993 (Wilson et al., 1994). Given the complexity of the problem, the experts made several assumptions: (1) the chemistry of Yucca Mountain groundwater is bounded by water from well J-13 and the Paleozoic aquifer (UE-25p#1), (2) the groundwater is oxidizing (which is expected to be conservative), and (3) it is necessary to model only far-field solubility because a precipitation front is expected in the far field, which will limit transport. However, it is anticipated that solubilities will differ within the canister from the far-field due to higher temperatures, lower silicic acid concentration, and variable Eh and pH values within the canister. It is important to know the solubility within the canister for criticality analysis and 10 CFR 60 release rate calculations. Examination of solubility values chosen by the expert panel suggests that they included conditions that we feel would be more typical within the canister and not likely to occur outside the canister. Therefore, a combination of values from TSPA-1993 and EQ3/6 simulations were used to estimate solubilities inside and outside the canisters. A more complete discussion of solubility can be found below, "Far-Field Solubility of Uranium, Plutonium, and Neptunium." Time restraints limited modeling to only silica concentrations in solution; however, future studies will include variations of Eh values.

Sorption is a function of water chemistry and rock type. We chose to use the simple K_d model, which assumes sorption is linear with concentration and is reversible. The distribution coefficient, K_d , a measure of the partitioning of a solute between the solid and aqueous phase (Cederberg, 1988), is the ratio of the activity of the sorbed specie on the solid phase per unit mass of solid (g/g) to the activity of the specie in solution per unit volume of solution (g/cm^3) (Cederberg, 1988). The K_d was used to place bounds on the expected sorption behavior. The larger the K_d value, the more solute is sorbed. The K_d distributions from TSPA-1993 (Wilson et al., 1994) were obtained from expert elicitation, also assuming a simple K_d model, and were grouped as follows: iron oxides (Fe), devitrified tuff (D), vitric tuff (V), and zeolitic tuff (Z). These groupings are based on the fact that the sorption of radionuclides is the result of a chemical reaction between the radionuclide in the groundwater and the minerals in the tuff. The K_d cumulative distributions used for the 1994 PA are reported in Table 5-14.

Far-Field Solubility of Uranium, Plutonium, and Neptunium. The most likely mechanism for a release of radionuclides to the environment is through waste-element dissolution into groundwater and transport to the accessible environment. The migration of radionuclides in groundwater is affected by chemical interactions between the groundwater and the aquifer material (host rock). Changes in groundwater chemistry can alter radionuclide concentrations and migration rates. The EQ3/6 geochemical modeling code package was used to simulate the chemical interactions between J-13 well water in the unsaturated zone of a welded devitrified tuff and the dissolution of high-level radioactive waste elements under oxidizing conditions. Most actinides are generally more soluble under oxidizing conditions; hence, results obtained under oxidizing conditions should be considered conservative. The unsaturated zone was conceptualized as an open system with O_2 and CO_2 in equilibrium with the atmosphere. The J-13 well water from the tuff aquifer was used to represent groundwater of the unsaturated zone near the proposed emplacement area. A saturation-limited model was used which is considered to be the most conservative modeling approach and which permits radionuclides in the water to reach maximum concentration limits. Results are presented from EQ3/6 modeling runs for radionuclides added as UO_2^{++} , Pu^{4+} , and Np^{4+} at temperatures of 25°C, 60°C, and 100°C, and input pH's of 5.9, 7, 8, and 9. Results include the main solution species, the controlling limiting phase, and solubilities for each radionuclide. The neptunium solubility was controlled by equilibrium with NpO_2 . The concentration of neptunium in solution decreased with increasing temperature and pH, but remained in a narrow range of solubility. Plutonium concentrations were controlled by the solubility-limiting phases $PuO_{2(c)}$ and $PuO_2(OH)_2$. Uranium solubility was controlled by the aqueous silica concentration and the formation of secondary uranium bearing precipitates.

Mineralogy of Tuff at the Repository Horizon. The repository rock was modeled after the Topopah Spring Tuff from the Yucca Mountain Project, which is a densely welded, devitrified tuff. High silica concentrations are associated with groundwaters leaching the tuff (Nitsche et al., 1993; Duffy, 1993). The silica content of the groundwaters is an important factor in limiting the concentration of radionuclides in solution (Bruton and Shaw, 1988; Bruton et al., 1991). The dominant minerals in Yucca Mountain are the silica polymorphs (tridymite, opal-CT, cristobalite, and quartz), clinoptilolite, sanidine, mordenite, analcime, and clays (Duffy, 1993). The three major phases—quartz, sanidine, and cristobalite—make up 98% of the host rock (Delany, 1985) (Table 11-3). Duffy hypothesized that the mineral transformations in Yucca Mountain are largely controlled by the decreasing aqueous silica activity caused by the evolution of the metastable silica polymorphs to quartz and the forms of solid SiO_2 are the regulating factors controlling the aqueous silica. The a_{SiO_2} is controlled by the solubility of the most soluble silica polymorph present (Duffy, 1993), and the a_{SiO_2} values change with temperature. It is assumed for this model that a_{SiO_2} must be above α -cristobalite saturation (Figure 11-5).

Table 11-3. Mineral Composition of Tuff from Topopah Spring Member of Paintbrush Tuff Formation (after Delany, 1985)

Mineral	Description	Composition	Volume (%)
Cristobolite (α, β)	a crystalline form of silica (SiO_2)	SiO_2	44
Sanidine	an alkali feldspar mineral rich in potassium	$(K, Na)AlSi_3O_8$	39
Quartz	the most common crystalline form of silica	SiO_2	14.9
Albite	a very common series of rock-forming minerals	$NaAlSi_3O_8$	1
Mg-beidellite	a member of the montmorillonite (smectite) group, rich in aluminum	$(Na, Ca_{0.5})_{0.3} (Al, Mg)_2 (Si, Al)_4 O_{10}(OH)_2$	1
Biotite	a common rock-forming mineral member of the mica group	$K(mg, Fe^{+2})_3 (Al, Fe^{+3}) Si_3O_{10}(OH)_2$	0.1
Total			100.0

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Figure 11-5. Silica content of waters from Yucca Mountain and surrounding area. Maximum solubility or range of solubility shown for several minerals composed of silicon dioxide (SiO_2). For example, shaded area represents the probable range of the solubility of opal- C^+ (form of silica). (From Kerrisk, 1984.)

Quartz silica has a very low solubility at ordinary temperatures and neutral pH of about 6 ppm of SiO_2 , and amorphous silica, the most unstable phase, dissolves to approximately 120 ppm (Krauskopf, 1979). The other forms of silica (opal, tridymite, cristobalite, chalcedony) have solubilities between these extremes. The different solubilities reflect the differences in stability of the various phases of silica. The silica assemblage of the tuff is composed of 44% cristobalite (Delany, 1985) and is modeled in the 1994 PA as β -cristobalite the most unstable silica phase (Figure 11-5). Silica phases more stable than α -cristobalite are suppressed using the suppress option in EQ3. This allows the solution to supersaturate with respect to the more unstable phases, (i.e., β -cristobalite).

Predictive Modeling with EQ3/6. Aqueous geochemistry of radionuclides is complex and a large number of stable and metastable solid phases affect the aqueous equilibrium concentrations of individual radionuclides. Factors that influence radionuclide behavior in the hydrogeologic environment are the solid phases and the solution species of respective radionuclides. The knowledge of solid phases and aqueous solution species helps in predicting radionuclide concentrations available for transport to the accessible environment. The purpose for solubility and speciation studies is to supply data for calculating radionuclide transport along potential pathways from the repository to the accessible environment. Solubility and speciation are functions of groundwater chemistry and, in turn, are used to define the source term for transport.

Predictive modeling using dissolution and precipitation of solid phases was used to estimate the geochemical processes affecting the solubility and speciation of selected radionuclides. EQ3/6 geochemical simulations of the dissolution of waste elements in the presence of groundwater in a tuffaceous rock were carried out to attempt to predict limits for radionuclide concentrations in solution and to identify the solubility limiting phases of potential radionuclide precipitates. A saturation-limited model (Kerrisk, 1984) was used, which permits radionuclide concentrations in the waters to reach maximum concentration limits.

Computer simulations yield:

- the sequence of solids precipitated; these solids are the limiting phases for dissolution of radionuclides,
- radionuclide concentrations in solution which are the solubilities of each respective radionuclide,
- aqueous solution species of radionuclides,
- the final pH and Eh of the solution at overall equilibrium.

The chemical model used to describe the system may not contain all the important mechanisms and processes that occur in a natural system. Any given problem might have several solutions. There are more plausible phases and mechanisms than there are linearly independent equations to describe the system.

EQ3/6. EQ3/6 is a geochemical modeling code package used to simulate interactions of groundwaters and solid phases in the natural environment. The software package release used was EQ3/6-V7-REL-V7.2a (Wolery and Daveler, 1992) for the UNIX platform. The code is composed of five parts (EQPT, EQ3NR, EQ6, XCON3, and XCON6). EQPT is the EQ3/6 data file preprocessor. Before running EQ3NR or EQ6, the preprocessor creates a set of DATA1 files from the DATA0 files supplied with the distribution package. EQ3NR and EQ6 are the two main FORTRAN computer codes and both use a common thermodynamic data base, DATA0.COM (see Figure 11-6). The thermodynamic data contained in the DATA0 file are processed through EQTL FORTRAN code that checks for mass and charge balance and writes the data files that are read directly by the EQ3NR and EQ6 source codes.

EQ3NR is a speciation-solubility code that produces a distribution of aqueous species, their thermodynamic activities, and saturation indices for various solids for the initial solution. EQ6 is used to compute the reaction path of the aqueous geochemical system by calculating changes in the rock-water-waste system as overall reaction progresses. The chemical evolution is driven by sets of irreversible and reversible reactions. The irreversible reactions represent the dissolution of the waste and the reversible precipitation of secondary minerals (limiting phases) and solution species. EQ6 is initialized by attaching a description of the aqueous solution generated from EQ3NR as an output PICKUP file (Wolery and Daveler, 1992). EQ6 output consists of the sequence of solution species, solid phases, and final pH and Eh of the solution.

Major limitations of EQ3/6 lie in the paucity and questionable accuracy of the available thermodynamic data. Predictions in this study apply only to overall equilibrium conditions. Experimental work of Bruton and Shaw (1988) and Delany and Wolery (1984) have helped to validate EQ3/6 as a geochemical modeling tool.

Simulation Input. Solubility simulations were done for uranium, neptunium, and plutonium. At this time, thermodynamic data are available in the EQ3/6 data base for only a few of the important waste elements. Analyses of J-13 well water were used to define the initial water composition for EQ3NR. The J-13 water is classified as a sodium bicarbonate type with high concentrations of silica (1×10^{-3} M), sodium, and bicarbonate ion (Nitsche et al., 1993). J-13 carbonate alkalinity is 2.34 meq/l, which corresponds to 142 ppm when calculated as HCO_3^- . The water is used as the reference because it produces from the same stratigraphic unit as that of the proposed repository (Harrar et al., 1990). Well water J-13 is expected to be as close as possible to the water of the repository horizon, and has been used in many experiments. J-13 groundwater analyses are reported in numerous publications; the values used for this study are taken from Nitsche et al. (1993) (see Table 11-4).

The primary process controlling evolution of the solution is mineral dissolution. Silica phases more stable than α -cristobolite are suppressed using the suppress option in EQ3, thereby imposing additional constraints on the initial solution. Because the aqueous silica concentration is 1×10^{-3} M in the J-13 water, the capacity for additional silica dissolution is only 1×10^{-3} M. The high silica concentrations are associated with groundwater leaching of tuff. An assumption was made that the high silica concentration could be maintained by adding additional silica to the system in EQ3/6 as a special reactant.

The geochemical environment modeled was defined as an open system to the atmosphere (Delany, 1985). Oxidizing conditions were assumed because present conditions indicate that the water in the unsaturated zone may be oxidizing (Wolfsberg et al., 1981). Fugacities of O_2 (g) and CO_2 (g) in the J-13 water were fixed at $10^{-0.7}$ and $10^{-3.5}$ bars respectively to simulate equilibrium with the atmosphere (Delany and Wolery, 1984).

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Figure 11-6. Flow diagram.

Table 11-4. Composition of Water in J-13 Well (from Nitsche et al., 1993)

Species	Concentration (mM)
Ca ⁺²	0.29
Mg ⁺²	0.072
Na ⁺	1.96
K ⁺	0.136
Li	0.009
Fe	0.0008
Mn	0.00002
Al ⁺³	0.0010
SiO ₂	1.07
F ⁻	0.11
Cl ⁻	0.18
SO ₄ ²⁻	0.19
NO ₃ ⁻	0.16
Total carbonate [H ₂ CO ₃ ⁺] + [HCO ₃ ⁻] + [CO ₃ ²⁻]	2.81
Total Alkalinity [HCO ₃ ⁻] + 2[CO ₃ ²⁻] + [OH ⁻] - [H ⁺]	2.34 meg/l or eg/m ³
pH	7.0
Eh	700 mV

Simulations between the fuel waste and J-13 water were run at temperatures of 25°C, 60°C, and 100°C at initial input pH of 5.9, 7, 8, and 9 at one atmosphere of pressure in the open system. The radionuclides were introduced to the solution in EQ6 as special reactants. Corrosion products from the container were not included in the simulations, although it is known that some of the canister corrosion products can decrease effective radionuclide solubilities by sorption.

Results. Results are presented for the solubility and speciation simulations for radionuclides added as UO₂⁺⁺, Pu⁴⁺, Np⁴⁺ in J-13 well water at three different temperatures (25°C, 60°C and 100°C) and four initial input pH values (5.9, 7, 8, 9). Simulations were made with (a) no suppression of stable silica phases (suppressed silica phases in the study include phases more stable than α-cristobalite), (b) no suppression of stable silica phases or PuO₂, (c) suppression of stable silica phases and PuO₂, and (d) suppression of stable silica phases and PuO₂, plus addition of silica as a special reactant. The additional silica was added because an assumption was made that silica concentration in solution would be depleted by precipitation of silicates. The term stable includes the phases quartz, tridymite, and chalcedony. Selected pH and temperature values were used to bracket the expected range of conditions by choosing parameters that represent the upper and lower limits anticipated for the system. Predictions made here cover:

1. the aqueous solution species for each radionuclide,
2. radionuclide solubilities, log (mM or mole/m³),
3. solid phases controlling solubility for each radionuclide,
4. final pH and Eh values of the system for each temperature and input pH.

The sequence of precipitates, concentrations of species in solution, and final pH and Eh values are shown in Appendix E.

Cumulative probability distributions were used for sampling radionuclide solubilities. The uncertainties in the groundwater composition require large ranges in input parameters. Possible variations in solution chemistry can result in order-of-magnitude changes in solubilities. The distributions consist of data obtained from EQ3/6 simulations and TSPA-1993 expert elicitation (see Table 11-5).

Table 11-5. Solubility Values and Cumulative Probability Distribution

Probability	0	0.1	0.9	1
Neptunium	-8.00	-6.57	-4.77	-2.00
Plutonium	-12.50	-9.00	-6.51	-5.00
Uranium	-8.60	-8.00	-3.75	-2.00

Neptunium EQ3/6 calculation values are shown to be $10^{-6.57}$ to $10^{-4.77}$ moles/l (Table 11-6). The values from expert elicitation for TSPA-1993 (10^{-8} and 10^{-2} moles/l) were used to bracket the limits for the neptunium solubility. The minimum solubility for plutonium was from EQ3/6 simulations, which put the lower limit at $10^{-12.5}$ moles/l. This value is 3-1/2 magnitudes below the minimum of 10^{-9} moles/l suggested by expert elicitation for TSPA-1993. The value of $10^{-6.51}$ moles/l was from EQ3/6 simulations and the 10^{-5} moles/l (one order of magnitude higher than TSPA-1993) was used to bracket the upper bound or maximum limit. Uranium solubilities differed by approximately one order of magnitude or less. EQ3/6 values used were $10^{-8.6}$ and $10^{-3.75}$ moles/l. The EQ3/6 value of $10^{-8.6}$ was used to bracket the lower limit of uranium solubility. The values 10^{-8} and 10^{-2} moles/l are from expert elicitation, and 10^{-2} was used to bracket the upper limit or maximum solubility of uranium.

Table 11-6. Solubilities for Elements in Logarithmic Space (moles/l) from EQ3/6

Element	Logarithm of minimum value	Logarithm of maximum value
Uranium	-8.60	-3.25
Plutonium	-12.60	-6.51
Neptunium	-6.57	-4.77

Uranium. The solubility of uranium was found to be highly sensitive to pH and temperature changes. The solubility of U^{+6} increased with the formation of carbonate species.

The initial solution pH is input in EQ3NR and does not remain fixed. As pH increases from the initial input and as the amount of CO_3^{2-} increases in solution, the solubility of uranium increases. An increase in CO_3^{2-} with increasing pH was noted by Nitsche et al., 1993 in experimental studies using J-13 well water. An inverse relationship was also noted between the concentration of uranium in solution and the concentration of aqueous silica (Figure 11-7). This relationship was described by Bruton and Shaw (1988). The uranium concentrations in solution and the identity of the uranium solid phases varied as a function of the SiO_2 concentration in solution (see also Bruton et al., 1991). Secondary U-bearing precipitates act as solubility limiting phases. The main solubility limiting phase in runs with stable silica phases suppressed and additional silica added as a reactant was soddyite $[(UO_2)_2(SiO_4) \cdot 2H_2O]$, a uranyl silicate. Schoepite ($UO_3 \cdot 2H_2O$), an oxide hydrate, and soddyite are the limiting phases with stable silica phases suppressed and no addition of silica as a special reactant. Soddyite/ $UO_2(OH)_2$ (beta) alternate as the dominant limiting

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Figure 11-7. Concentration of radionuclides vs fixed amount of SiO_2 in solution (H_4SiO_4). Plots show that as silica in solution is depleted due to reaction with uranium to form uranyl silicate solids. The solubility of uranium increases.

phase in the no-suppression silica runs. Carbonate species [$\text{UO}_2(\text{CO}_3)_2(\text{aq})$, $\text{UO}_2(\text{CO}_3)_2^{--}$, $\text{UO}_2(\text{CO}_3)_3^{---}$] in solution were dominating throughout the pH range of 7 to 9. The formation of the mixed complex $(\text{UO}_2)_2\text{CO}_3(\text{OH})_3^-$ is found at 25°C as the silica is depleted from the system.

The uranium solubility range with aqueous silica concentration maintained in the solution ranged from $10^{-8.6}$ to $10^{-7.41}$ moles/l. When aqueous silica was depleted in the solution the uranium solubility ranged from $10^{-7.14}$ to $10^{-4.38}$ moles/l. The range was extended one order of magnitude due to uncertainty in the silica concentration to $10^{-3.25}$ moles/l as a maximum solubility for calculations. The TSPA-1993 reported solubilities elicited from experts based on their opinions on empirical data, primarily from laboratory measurements. Uranium ranged from 10^{-8} to 10^{-2} moles/l in TSPA-1993. The solubilities for uranium (with stable silica phases suppressed plus α -cristobalite added as a reactant and with no suppression of stable silica phases) modeled with EQ3/6 lie within the range obtained by expert elicitation for TSPA-1993. The cumulative distribution for uranium takes into account the uncertainty in the aqueous silica concentration with time.

Plutonium. Plutonium was modeled with and without $\text{PuO}_2(\text{c})$ suppression. Under oxic conditions and no suppression the solubility of plutonium was controlled by equilibrium with $\text{PuO}_2(\text{c})$; with suppression, the solubility was controlled by $\text{PuO}_2(\text{OH})_2$. Experimental work by Nitsche et al. (1993) indicated the formation of crystalline $\text{PuO}_2(\text{c})$ did not occur due to the time restraint of the experiments of less than 140 days. $\text{PuO}_2(\text{c})$ suppressed in EQ3 allowed for the slow formation of $\text{PuO}_2(\text{c})$ by keeping plutonium species in solution. Plutonium was also modeled without suppressing $\text{PuO}_2(\text{c})$ assuming in the far-field there would be sufficient time for $\text{PuO}_2(\text{c})$ to precipitate. The difference found in solubilities between suppression and no suppression of $\text{PuO}_2(\text{c})$ was approximately 4 orders of magnitude for the lower and upper boundaries.

The range for the 1994 PA calculations obtained from EQ3/6 was $10^{-12.5}$ to $10^{-6.51}$ moles/l. Extremely low solubilities were found for plutonium without suppression of $\text{PuO}_2(\text{c})$ in the range of $10^{-12.5}$ to $10^{-10.0}$ moles/l, and $10^{-8.5}$ to $10^{-6.51}$ moles/l when $\text{PuO}_2(\text{c})$ was suppressed. $\text{Pu}(\text{OH})_5^-$, $\text{PuO}_2\text{OH}(\text{aq})$, $\text{PuO}_2(\text{CO}_3)_2^{--}$, PuO_2^+ were the primary aqueous species under different Eh-pH conditions (see Appendix E). The extremely low solubilities (e.g. $10^{-12.5}$ moles/l) for plutonium are in agreement with studies by Allard (1982) and work by Wilson (1989). Plutonium disso-

lution was found to be greatest at 100°C, with no trend noted with pH changing from initial input (in agreement with Nitsche et al., 1993). The uncertainty in the formation of $\text{PuO}_2(\text{c})$ and the possible formation of plutonium colloids necessitated using TSPA-1993 range of $10^{-10.0}$ to $10^{-6.0}$ moles/l obtained from expert elicitation to increase the maximum boundary. This maximum boundary was increased by one order of magnitude to 10^{-5} moles/l by analyst decision due to uncertainty.

Neptunium. The solubility limiting solid was determined to be $\text{NpO}_2(\text{s})$ for all conditions. The carbonate complexation in solution (as noted with uranium) increased with increasing pH and temperature. (See Appendix E for species in solution.) The assumption of a fixed O_2 fugacity may overestimate the Np concentration in solution. Np concentrations are shown to be highly dependent on O_2 fugacity (Bruton et al., 1991). Neptunium solubility decreased with increasing temperature. A decrease in solubility was noted in experimental work by Nitsche et al. (1993) and was connected to an increase in the formation of CO_3^{2-} with increasing pH.

The neptunium solubility for EQ3/6 ranged from a low of $10^{-6.8}$ to $10^{-4.8}$ moles/l. The TSPA-1993 range was 10^{-8} to 10^{-2} moles/l. For the cumulative distribution for neptunium the uncertainty in the effect of fixed O_2 fugacity and silica concentration required using TSPA-1993 values to bound possible limits. The effect of neptunyl silicates is unknown at present, and none is included in the thermodynamic data base.

Conclusions. Results for the geochemical simulations are dependent on the completeness of the thermodynamic database. Initial results suggest:

- Soddyite and schoepite are the main uranium bearing precipitates. These phases will act as limiting phases for UO_2 solubility.
- An inverse relationship exists between the uranium concentration in solution and aqueous silica concentration in solution. This relationship is more fully explained in Bruton and Shaw (1988). The uranium concentrations in solution and the identity of the uranium solid phases vary as a function of the SiO_2 concentration in solution.
- The uranium dissolution is suppressed when aqueous silica remains at concentrations sufficient to support precipitation of uranyl silicates.
- Uranium concentrations vary significantly with temperature and pH.
- Increasing temperature has little effect on the identity of the limiting phase precipitates.
- Precipitated phases for neptunium and plutonium are oxides of the elements.
- Neptunium solubility decreased with increasing temperature and input pH.

The results for the above radionuclides are in good agreement with a study by Wilson and Bruton (1989).

Future work should include:

- Modeling runs with oxygen limited. With low O_2 levels Pu^{3+} becomes stable, increasing solubility. Neptunium concentrations in solution should be dependent on oxygen fugacity.
- Varying the pCO_2 to greater than $10^{-3.5}$ atmospheres. At depth the partial pressure may exceed $10^{-3.5}$.
- Further work with Eh dependence.

11.4 Summary of Modeling Parameters

Tables 11-7, 11-8, and 11-9 summarize the modeling parameters used by GASSNF and USATCONC for the waste parcels, elements, and radionuclides, respectively. The parameters for the 1994 PA were of necessity chosen in a very short period of time. An exhaustive review of the literature was not possible; instead, recent literature, review articles, and personal communications with various experts were used as guidance in making educated guesses.

Table 11-7. Modeling Parameters for the Waste Emplacement Packages

Parameter	Description	Median	Low Range	High Range	Units	Distribution
AL – Aluminium						
COR_A_HO	Corrosion term A for humid oxic cond.	2.36e+18			kg/m ² s	CONSTANT
COR_A_WO	Corrosion term A for wet oxic cond.	2.00e-08			kg/m ² s	CONSTANT
COR_B_HO	Corrosion term B for humid oxic cond.	2.20e+04			K	CONSTANT
COR_B_WO	Corrosion term B for wet oxic cond.	0			K	CONSTANT
COR_C_HO	Corrosion term C for humid oxic cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxic cond.	1			none	CONSTANT
CORMOD	Corrosion mode	0			none	CONSTANT
FRCPENHO	Penetration fraction under humid oxic cond.	5.00e-01			none	CONSTANT
FRCPENWO	Fraction removed at penetration, wet oxic cond.	5.00e-01			none	CONSTANT
MW	Molecular weight	27			g/mole	CONSTANT
SGAS_HO	Stoichiometry for gas phase under humid cond.	-7.50e-01			none	CONSTANT
SGAS_WO	Stoichiometry for gas phase under oxic cond.	-7.50e-01			none	CONSTANT
SH2O_HO	Stoichiometry for water under humid cond.	0			none	CONSTANT
SH2O_WO	Stoichiometry for water under oxic cond.	0			none	CONSTANT
SRUST	Stoichiometry for rust formed	0			none	CONSTANT
BSTEELNP – Borated Steel-Nonprotecting, see SS304LP						
BSTEELP – Borated Steel-Protecting, see SS304LP						
CALCINE – Calcine						
COR_A_HO	Corrosion term A for humid oxic cond.	0			none	CONSTANT
COR_A_WO	Corrosion term A for wet oxic cond.	4.00e-07			1/s	CONSTANT
COR_B_HO	Corrosion term B for humid oxic cond.	0			none	CONSTANT
COR_B_WO	Corrosion term B for wet oxic cond.	0			1/s	CONSTANT

Table 11-7. Modeling Parameters for the Waste Emplacement Packages (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
COR_C_HO	Corrosion term C for humid oxid cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxid cond.	1			none	CONSTANT
CORMOD	Corrosion mode	1			none	CONSTANT
CSTEEL – Carbon Steel, ASTM Grade 516						
COR_A_HO	Corrosion term A for humid oxid cond.	4.73			kg/m ² s	CONSTANT
COR_A_WO	Corrosion term A for wet oxid cond.	9.49e-05	3.00e-05	3.00e-04	kg/m ² s	LOGUNIFORM
COR_B_HO	Corrosion term B for humid oxid cond.	6.87e+03			K	CONSTANT
COR_B_WO	Corrosion term B for wet oxid cond.	2.53e+03			K	CONSTANT
COR_C_HO	Corrosion term C for humid oxid cond.	3.30e-01			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxid cond.	1			none	CONSTANT
CORMOD	Corrosion mode	0			none	CONSTANT
FRCPENHO	Penetration fraction under humid oxid cond.	9.00e-01			none	CONSTANT
FRCPENWO	Penetration fraction under wet oxid cond.	1.00e-01			none	CONSTANT
MW	Molecular weight	55.9			g/mole	CONSTANT
SGAS_HO	Stoichiometry for gas phase under humid cond.	-3.30e-01			none	CONSTANT
SGAS_WO	Stoichiometry for gas phase under oxid cond.	-3.30e-01			none	CONSTANT
SH2O_HO	Stoichiometry for water under humid cond.	0			none	CONSTANT
SH2O_WO	Stoichiometry for water under oxid cond.	0			none	CONSTANT
SRUST	Stoichiometry for rust formed	1			none	CONSTANT
CERAMIC – Ceramic Phase of Glass-ceramic Waste Form						
COR_A_HO	Corrosion term A for humid oxid cond.	0			none	CONSTANT
COR_A_WO	Corrosion term A for wet oxid cond.	1.00e-14	1.00e-17	1.00e-11	kg/m ² s	LOGUNIFORM
COR_B_HO	Corrosion term B for humid oxid cond.	0			none	CONSTANT
COR_B_WO	Corrosion term B for wet oxid cond.	0			K	CONSTANT

Table 11-7. Modeling Parameters for the Waste Emplacement Packages (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
COR_C_HO	Corrosion term C for humid oxid cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxid cond.	1			none	CONSTANT
CORMOD	Corrosion mode	0			none	CONSTANT
GLASS – Borosilicate Glass Waste Form or Glass Phase of Glass-ceramic Waste Form						
COR_A_HO	Corrosion term A for humid oxid cond.	0			none	CONSTANT
COR_A_WO	Corrosion term A for wet oxid cond.	1.00e-10	1.00e-12	1.00e-08	kg/m ² s	LOGUNIFORM
COR_B_HO	Corrosion term B for humid oxid cond.	0			none	CONSTANT
COR_B_WO	Corrosion term B for wet oxid cond.	0			K	CONSTANT
COR_C_HO	Corrosion term C for humid oxid cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxid cond.	1			none	CONSTANT
CORMOD	Corrosion mode	0			none	CONSTANT
GRAPHITE – Graphite						
COR_A_HO	Corrosion term A for humid oxid cond.	4.79e+01			kg/m ² s	CONSTANT
COR_A_WO	Corrosion term A for wet oxid cond.	4.79e+01			kg/m ² s	CONSTANT
COR_B_HO	Corrosion term B for humid oxid cond.	1.72e+04			K	CONSTANT
COR_B_WO	Corrosion term B for wet oxid cond.	1.72e+04			K	CONSTANT
COR_C_HO	Corrosion term C for humid oxid cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxid cond.	1			none	CONSTANT
CORMOD	Corrosion mode	0			none	CONSTANT
FRCPENHO	Penetration fraction under humid oxid cond.	0			none	CONSTANT
FRCPENWO	Penetration fraction under wet oxid cond.	0			none	CONSTANT
MW	Molecular weight	12			g/mole	CONSTANT
SGAS_HO	Stoichiometry for gas phase under humid cond.	-1			none	CONSTANT
SGAS_WO	Stoichiometry for gas phase under oxid cond.	-1			none	CONSTANT

Table 11-7. Modeling Parameters for the Waste Emplacement Packages (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
SH2O_HO	Stoichiometry for water under humid cond.	0			none	CONSTANT
SH2O_WO	Stoichiometry for water under oxidic cond.	0			none	CONSTANT
SRUST	Stoichiometry for rust formed	0			none	CONSTANT
IN825 – Incoloy 825						
COR_A_HO	Corrosion term A for humid oxidic cond.	4.56e-03			kg/m ² s	CONSTANT
COR_A_WO	Corrosion term A for wet oxidic cond.	5.60e+14	5.60e+13	5.60e+15	kg/m ² s	LOGUNIFORM
COR_B_HO	Corrosion term B for humid oxidic cond.	1.32e+04			K	CONSTANT
COR_B_WO	Corrosion term B for wet oxidic cond.	1.96e+04			K	CONSTANT
COR_C_HO	Corrosion term C for humid oxidic cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxidic cond.	1			none	CONSTANT
CORMOD	Corrosion mode	0			none	CONSTANT
FRCPENHO	Penetration fraction under humid oxidic cond.	3.00e-02			none	CONSTANT
FRCPENWO	Penetration fraction under wet oxidic cond.	3.00e-02			none	CONSTANT
MW	Molecular weight	57			g/mole	CONSTANT
SGAS_HO	Stoichiometry for gas phase under humid cond.	-5.30e-01			none	CONSTANT
SGAS_WO	Stoichiometry for gas phase under oxidic cond.	-5.30e-01			none	CONSTANT
SH2O_HO	Stoichiometry for water under humid cond.	0			none	CONSTANT
SH2O_WO	Stoichiometry for water under oxidic cond.	0			none	CONSTANT
SRUST	Stoichiometry for rust formed	3.10e-01			none	CONSTANT
MC2 – Metal Carbide						
COR_A_HO	Corrosion term A for humid oxidic cond.	1.00e-09			1/s	CONSTANT
COR_A_WO	Corrosion term A for wet oxidic cond.	1.00e-09			1/s	CONSTANT
COR_B_HO	Corrosion term B for humid oxidic cond.	0			K	CONSTANT
COR_B_WO	Corrosion term B for wet oxidic cond.	0			K	CONSTANT

Table 11-7. Modeling Parameters for the Waste Emplacement Packages (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
COR_C_HO	Corrosion term C for humid oxic cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxic cond.	1			none	CONSTANT
CORMOD	Corrosion mode	1			none	CONSTANT
FRCPENHO	Penetration fraction under humid oxic cond.	0			none	CONSTANT
FRCPENWO	Penetration fraction under wet oxic cond.	0			none	CONSTANT
MW	Molecular weight	2.56e+02			g/mole	CONSTANT
SGAS_HO	Stoichiometry for gas phase under humid cond.	2			none	CONSTANT
SGAS_WO	Stoichiometry for gas phase under oxic cond.	2			none	CONSTANT
SH2O_HO	Stoichiometry for water under humid cond.	2			none	CONSTANT
SH2O_WO	Stoichiometry for water under oxic cond.	2			none	CONSTANT
SRUST	Stoichiometry for rust formed	0			none	CONSTANT
RUST – Rust						
MW	Molecular weight	79.8			g/mole	CONSTANT
SS304LNP – Stainless Steel 304L-Nonprotecting, see SS304LP						
SS304LP – Stainless Steel 304L-Protecting						
COR_A_HO	Corrosion term A for humid oxic cond.	1.00e-13	1.00e-16	1.00e-10	kg/m ² s	LOGUNIFORM
COR_A_WO	Corrosion term A for wet oxic cond.	1.00e-13	1.00e-16	1.00e-10	kg/m ² s	LOGUNIFORM
COR_B_HO	Corrosion term B for humid oxic cond.	0			K	CONSTANT
COR_B_WO	Corrosion term B for wet oxic cond.	0			K	CONSTANT
COR_C_HO	Corrosion term C for humid oxic cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxic cond.	1			none	CONSTANT
CORMOD	Corrosion mode	0			none	CONSTANT
FRCPENHO	Penetration fraction under humid oxic cond.	0			none	CONSTANT
FRCPENWO	Penetration fraction under wet oxic cond.	0			none	CONSTANT

Table 11-7. Modeling Parameters for the Waste Emplacement Packages (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
MW	Molecular weight	53.2			g/mole	CONSTANT
SGAS_HO	Stoichiometry for gas phase under humid cond.	-4.30e-01			none	CONSTANT
SGAS_WO	Stoichiometry for gas phase under oxic cond.	-4.30e-01			none	CONSTANT
SH2O_HO	Stoichiometry for water under humid cond.	0			none	CONSTANT
SH2O_WO	Stoichiometry for water under oxic cond.	0			none	CONSTANT
SRUST	Stoichiometry for rust formed	7.00e-01			none	CONSTANT
TRISO – TRISO Coating for MC2						
COR_A_HO	Corrosion term A for humid oxic cond.	3.00e-11	3.00e-12	3.00e-10	1/s	LOGUNIFORM
COR_A_WO	Corrosion term A for wet oxic cond.	3.00e-11	3.00e-12	3.00e-10	1/s	LOGUNIFORM
COR_B_HO	Corrosion term B for humid oxic cond.	0			K	CONSTANT
COR_B_WO	Corrosion term B for wet oxic cond.	0			K	CONSTANT
COR_C_HO	Corrosion term C for humid oxic cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxic cond.	1			none	CONSTANT
CORMOD	Corrosion mode	1			none	CONSTANT
FRCPENHO	Penetration fraction under humid oxic cond.	1			none	CONSTANT
FRCPENWO	Penetration fraction under wet oxic cond.	1			none	CONSTANT
MW	Molecular weight	40.1			g/mole	CONSTANT
SGAS_HO	Stoichiometry for gas phase under humid cond.	0			none	CONSTANT
SGAS_WO	Stoichiometry for gas phase under oxic cond.	0			none	CONSTANT
SH2O_HO	Stoichiometry for water under humid cond.	0			none	CONSTANT
SH2O_WO	Stoichiometry for water under oxic cond.	0			none	CONSTANT
SRUST	Stoichiometry for rust formed	0			none	CONSTANT
U – Uranium						
COR_A_HO	Corrosion term A for humid oxic cond.	1.35e+02			kg/m ² s	CONSTANT

Table 11-7. Modeling Parameters for the Waste Emplacement Packages (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
COR_A_WO	Corrosion term A for wet oxic cond.	9.40e+03			kg/m ² ss	CONSTANT
COR_B_HO	Corrosion term B for humid oxic cond.	7.24e+03			K	CONSTANT
COR_B_WO	Corrosion term B for wet oxic cond.	7.97e+03			K	CONSTANT
COR_C_HO	Corrosion term C for humid oxic cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxic cond.	1			none	CONSTANT
CORMOD	Corrosion mode	0			none	CONSTANT
FRCPENHO	Penetration fraction under humix oxic cond.	0			none	CONSTANT
FRCPENWO	Penetration fraction under wet oxic cond.	0			none	CONSTANT
MW	Molecular weight	2.38e+02			g/mole	CONSTANT
SGAS_HO	Stoichiometry for gas phase under humid cond.	-1.50			none	CONSTANT
SGAS_WO	Stoichiometry for gas phase under oxic cond.	-1.50			none	CONSTANT
SH2O_HO	Stoichiometry for water under humid cond.	-2			none	CONSTANT
SH2O_WO	Stoichiometry for water under oxic cond.	2			none	CONSTANT
SRUST	Stoichiometry for rust formed	0			none	CONSTANT
UALX – Uranium Aluminide						
COR_A_HO	Corrosion term A for humid oxic cond.	1.35e+02			kg/m ² s	CONSTANT
COR_A_WO	Corrosion term A for wet oxic cond.	2.00e-06			kg/m ² s	CONSTANT
COR_B_HO	Corrosion term B for humid oxic cond.	7.24e+03			K	CONSTANT
COR_B_WO	Corrosion term B for wet oxic cond.	0			K	CONSTANT
COR_C_HO	Corrosion term C for humid oxic cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxic cond.	1			none	CONSTANT
CORMOD	Corrosion mode	0			none	CONSTANT
FRCPENHO	Penetration fraction under humix oxic cond.	0			none	CONSTANT
FRCPENWO	Penetration fraction under wet oxic cond.	0			none	CONSTANT

Table 11-7. Modeling Parameters for the Waste Emplacement Packages (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
MW	Molecular weight	3.22e+02			g/mole	CONSTANT
SGAS_HO	Stoichiometry for gas phase under humid cond.	-3.90			none	CONSTANT
SGAS_WO	Stoichiometry for gas phase under oxid cond.	-3.90			none	CONSTANT
SH2O_HO	Stoichiometry for water under humid cond.	0			none	CONSTANT
SH2O_WO	Stoichiometry for water under oxid cond.	0			none	CONSTANT
SRUST	Stoichiometry for rust formed	0			none	CONSTANT
UO₂ – Uranium Dioxide						
COR_A_HO	Corrosion term A for humid oxid cond.	1.70e-04			kg/m ² s	CONSTANT
COR_A_WO	Corrosion term A for wet oxid cond.	4.43e-06	1.40e-07	1.40e-04	kg/m ² s	LOGUNIFORM
COR_B_HO	Corrosion term B for humid oxid cond.	5.90e+03			K	CONSTANT
COR_B_WO	Corrosion term B for wet oxid cond.	3.61e+03			K	CONSTANT
COR_C_HO	Corrosion term C for humid oxid cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxid cond.	1			none	CONSTANT
CORMOD	Corrosion mode	0			none	CONSTANT
WATER – Groundwater						
MW	Molecular weight	18			g/mole	CONSTANT
ZIRCALOY – Zircaloy						
COR_A_HO	Corrosion term A for humid oxid cond.	6.00e-02			kg/m ² s	CONSTANT
COR_A_WO	Corrosion term A for wet oxid cond.	1.00e-12			kg/m ² s	CONSTANT
COR_B_HO	Corrosion term B for humid oxid cond.	1.12e+04			K	CONSTANT
COR_B_WO	Corrosion term B for wet oxid cond.	0			K	CONSTANT
COR_C_HO	Corrosion term C for humid oxid cond.	1			none	CONSTANT
COR_C_WO	Corrosion term C for wet oxid cond.	1			none	CONSTANT
CORMOD	Corrosion mode	0			none	CONSTANT

Table 11-7. Modeling Parameters for the Waste Emplacement Packages (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
FRCPENHO	Penetration fraction under humix oxic cond.	1.00e-01			none	CONSTANT
FRCPENWO	Penetration fraction under wet oxic cond.	1.00e-01			none	CONSTANT
MW	Molecular weight	91.2			g/mole	CONSTANT
SGAS_HO	Stoichiometry for gas phase under humid cond.	-1			none	CONSTANT
SGAS_WO	Stoichiometry for gas phase under oxic cond.	-1			none	CONSTANT
SH2O_HO	Stoichiometry for water under humid cond.	0			none	CONSTANT
SH2O_WO	Stoichiometry for water under oxic cond.	1			none	CONSTANT
SRUST	Stoichiometry for rust formed	0			none	CONSTANT
WEP101 – Graphite Spent Fuel in USF-MPC						
ECFF	Early clad failure fraction	4.50e-02	3.70e-02	5.30e-02	none	UNIFORM
WEP102 – N-Reactor Spent Fuel in USF_MPC						
ECFF	Early clad failure fraction	3.30e-01	1.60e-01	5.00e-01	none	UNIFORM
QRF_M1C	Quick release fraction of C14 in matrix 1	2.00e-02			none	CONSTANT
WEP103 – Shippingport Spent Fuel in USF-MPC						
ECFF	Early clad failure fraction	1.00e-02	1.00e-03	1.00e-01	none	LOGUNIFORM
QRF_M1C	Quick release fraction of C14 in matrix 1	2.00e-02			none	CONSTANT
QRF_M2C	Quick release fraction of C14 in matrix 2	1.30e-01	1.00e-02	2.50e-01	none	UNIFORM
QRF_M2CS	Quick release fraction of Cs in matrix 2	8.10e-02	5.77e-02	1.04e-01	none	NORMAL
QRF_M2I	Quick release fraction of I129 in matrix 2	8.10e-02	5.77e-02	1.04e-01	none	NORMAL
QRF_M2TC	Quick release fraction of Tc99 in matrix 2	6.00e-02	3.67e-02	8.33e-02	none	NORMAL
WEP104 – ATR (HEU) Spent Fuel in USF-MPC						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP105 – Commercial PWR (LEU) Spent Fuel in PWR-MPC						
ECFF	Early clad failure fraction	1.00e-02	1.00e-03	1.00e-01	none	LOGUNIFORM

Table 11-7. Modeling Parameters for the Waste Emplacement Packages (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
QRF_M1C	Quick release fraction of C14 in matrix 1	2.00e-02			none	CONSTANT
QRF_M2C	Quick release fraction of C14 in matrix 2	1.30e-01	1.00e-02	2.50e-01	none	UNIFORM
QRF_M2CS	Quick release fraction of Cs in matrix 2	8.10e-02	5.77e-02	1.04e-01	none	NORMAL
QRF_M2I	Quick release fraction of I129 in matrix 2	8.10e-02	5.77e-02	1.04e-01	none	NORMAL
QRF_M2TC	Quick release fraction of Tc99 in matrix 2	6.00e-02	3.67e-02	8.33e-02	none	NORMAL
WEP106 – Calcine HLW Glass-ceramic in BHLW-MPC						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP107 – DWPP HLW Borosilicate Glass in BHLW-MPC						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP108 – HWVP HLW Borosilicate in DHLW-MPC						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP109 – WVDP HLW Borosilicate Glass in DHLW-MPC						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP110 – Calcine HLW Borosilicate Glass in DHLW-MPC						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP111 – Calcine HLW Loose in DHLW-MPC						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP201 – Graphite Spent Fuel in LWT Cask						
ECFF	Early clad failure fraction	4.50e-02	3.70e-02	5.30e-02	none	UNIFORM
WEP202 – N-Reactor Spent Fuel in LWT Cask						
ECFF	Early clad failure fraction	3.30e-01	1.60e-01	5.00e-01	none	UNIFORM
QRF_M1C	Quick release fraction of C14 in matrix 1	2.00e-02			none	CONSTANT

Table 11-7. Modeling Parameters for the Waste Emplacement Packages (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
WEP203 – Shippingport Spent Fuel in LWT Cask						
ECFF	Early clad failure fraction	1.00e-02	1.00e-03	1.00e-01	none	LOGUNIFORM
QRF_M1C	Quick release fraction of C14 in matrix 1	2.00e-02			none	CONSTANT
QRF_M2C	Quick release fraction of C14 in matrix 2	1.30e-01	1.00e-02	2.50e-01	none	UNIFORM
QRF_M2CS	Quick release fraction of Cs in matrix 2	8.10e-02	5.77e-02	1.04e-01	none	NORMAL
QRF_M2I	Quick release fraction of I129 in matrix 2	8.10e-02	5.77e-02	1.04e-01	none	NORMAL
QRF_M2TC	Quick release fraction of Tc99 in matrix 2	6.00e-02	3.67e-02	8.33e-02	none	NORMAL
WEP204 – ATR (HEU) Spent Fuel in LWT Cask						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP205 – Commercial PWR (LEU) Spent Fuel in LWT Cask						
ECFF	Early clad failure fraction	1.00e-02	1.00e-03	1.00e-01	none	LOGUNIFORM
QRF_M1C	Quick release fraction of C14 in matrix 1	2.00e-02			none	CONSTANT
QRF_M2C	Quick release fraction of C14 in matrix 2	1.30e-01	1.00e-02	2.50e-01	none	UNIFORM
QRF_M2CS	Quick release fraction of Cs in matrix 2	8.10e-02	5.77e-02	1.04e-01	none	NORMAL
QRF_M2I	Quick release fraction of I129 in matrix 2	8.10e-02	5.77e-02	1.04e-01	none	NORMAL
QRF_M2TC	Quick release fraction of Tc99 in matrix 2	6.00e-02	3.67e-02	8.33e-02	none	NORMAL
WEP206 – Calcline HLW glass-ceramic in DOE "Standard" Canister						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP207 – DWPP HLW Borosilicate Glass in DOE "Standard" Canister						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP208 – HWVP HLW Borosilicate in DOE "Standard" Canister						
ECFF	Early clad failure fraction	0			none	CONSTANT

Table 11-7. Modeling Parameters for the Waste Emplacement Packages (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
WEP209 – WVDP HLW Borosilicate Glass in DOE "Standard" Canister						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP210 – Calcine HLW Borosilicate Glass in DOE "Standard" Canister						
ECFF	Early clad failure fraction	0			none	CONSTANT
WEP211 – Calcine HLW Loose in DOE "Standard" Canister						
ECFF	Early clad failure fraction	0			none	CONSTANT
CANISTER – Canister						
BACFRC	Fraction of WEPs with backfill or rubble	5.00e-01	0	1	none	UNIFORM
EBFRAC	Juvenile failure fraction of outer layer of WEPs	5.00e-03	0	1.00e-02	none	UNIFORM
EFFCAREA	Factor for effective collection area of WEPs	0	-5.00e-01	5.00e-01	none	UNIFORM
EFFDAREA	Effective diffusion area/tortuosity for WEPs	1.00e-03	1.00e-06	1	none	LOGUNIFORM
FRACTURE – Fracture						
S99A	Fracture saturation where corrosion is 99% of flooded rate, intact air gap WEPs)	8.00e-02			none	CONSTANT
S99B	Fracture saturation where corrosion is 99% of flooded rate, rubble/backfill WEPs)	8.00e-02			none	CONSTANT
TSA	Threshold fracture saturation for wet corrosion, intact air gap WEPs	4.00e-02			none	CONSTANT
TSB	Threshold fracture saturation for wet corrosion, backfill/rubble WEPs	0			none	CONSTANT

Table 11-8. Modeling Parameters for Elements

Parameter	Description	Median	Low Range	High Range	Units	Distribution
AC – Actinium						
LOGSOLM	Elicited log solubility for elements	-8.00e+000	-1.00e+001	-6.00e+000	moles/l	UNIFORM
AM – Americium						
LOGSOLM	Elicited log solubility for elements	-8.00e+000	-1.00e+001	-6.00e+000	moles/l	UNIFORM
C – Carbon Element						
KDI	Intercept of C14 KD curve	4.60e+001	none	CONSTANT		
KDS	Slope of C14 KD curve	-4.75e-001	none	CONSTANT		
LOGSOLM	Elicited log solubility for elements	1.00e+000	moles/l	CONSTANT		
LOGSOLMS	Log of solubility for silic oxic conditions	1.00e+000	moles/l	CONSTANT		
CL – Chlorine						
LOGSOLM	Elicited log solubility for elements	00.00e+001	moles/l	CONSTANT		
CS – Cesium						
LOGSOLM	Elicited log solubility for elements	00.00e+001	moles/l	CONSTANT		
I – Iodine						
LOGSOLM	Elicited log solubility for elements	00.00e+001	moles/l	CONSTANT		
NB – Niobium						
LOGSOLM	Elicited log solubility for elements	-8.00e+000	-9.00e+000	-7.00e+000	moles/l	UNIFORM
NI – Nickel						
LOGSOLM	Elicited log solubility for elements	-2.70e+000	-6.00e+000	-1.00e+000	moles/l	BETA
NP – Neptunium						
LOGSOLM	Elicited log solubility for elements	-3.94e+000	-8.00e+000	-2.00e+000	moles/l	BETA
LOGSOLMS	Log of solubility for silic oxic conditions	-5.67e+000	-8.00e+000	-2.00e+000	moles/l	CUMULATIVE

Table 11-8. Modeling Parameters for Elements (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
PA – Protactinium						
LOGSOLM	Elicited log solubility for elements	-7.50e+000	-1.00e+001	-5.00e+000	moles/l	UNIFORM
LOGSOLMS	Log of solubility for silic oxic conditions	-7.50e+000	-1.00e+001	-5.00e+000	moles/l	UNIFORM
PB – Lead						
LOGSOLM	Elicited log solubility for elements	-6.50e+000	-8.00e+000	-5.00e+000	moles/l	BETA
PU – Plutonium						
LOGSOLM	Elicited log solubility for elements	-8.00e+000	-1.00e+001	-6.00e+000	moles/l	UNIFORM
LOGSOLMS	Log of solubility for silic oxic conditions	-7.75e+000	-1.25e+001	-5.00e+000	moles/l	CUMULATIVE
RA – Radium						
LOGSOLM	Elicited log solubility for elements	-7.00e+000	-9.00e+000	-5.00e+000	moles/l	BETA
SE – Selenium						
LOGSOLM	Elicited log solubility for elements	00.00e+001	moles/l	CONSTANT		
SM – Samarium						
LOGSOLM	Elicited log solubility for elements	-8.00e+000	-1.00e+001	-6.00e+000	moles/l	UNIFORM
SN – Tin						
LOGSOLM	Elicited log solubility for elements	-9.00e+000	-1.10e+001	-7.00e+000	moles/l	UNIFORM
SR – Strontium						
LOGSOLM	Elicited log solubility for elements	-3.95e+000	-6.00e+000	-3.00e+000	moles/l	BETA
TC – Technetium						
LOGSOLM	Elicited log solubility for elements	00.00e+001	moles/l	CONSTANT		
TH – Thorium						
LOGSOLM	Elicited log solubility for elements	-8.50e+000	-1.00e+001	-7.00e+000	moles/l	UNIFORM

Table 11-8. Modeling Parameters for Elements (Continued)

Parameter	Description	Median	Low Range	High Range	Units	Distribution
U – Uranium						
LOGSOLM	Elicited log solubility for elements	-4.46e+000	-8.00e+000	-2.00e+000	moles/l	BETA
LOGSOLMS	Log of solubility for silic oxic conditions	-5.62e+000	-8.60e+000	-2.00e+000	moles/l	CUMULATIVE
ZR – Zirconium						
LOGSOLM	Elicited log solubility for elements	-9.50e+000	-1.20e+001	-7.00e+000	moles/l	UNIFORM

Table 11-9. Modeling Parameters for the Radionuclides

Parameter*	Value	Units	Parameter*	Value	Units
AM241 – Americium 241			AM243 – Americium 243		
HALFLIFE	1.36e+010	Seconds	HALFLIFE	2.32e+011	Seconds
INVWP101	2.26e+001	Ci	INVWP101	1.75e-001	Ci
INVWP102	2.72e+003	Ci	INVWP102	5.06e-001	Ci
INVWP103	7.01e+002	Ci	INVWP103	2.99e+000	Ci
INVWP104	6.60e+002	Ci	INVWP104	4.13e-001	Ci
INVWP105	1.73e+004	Ci	INVWP105	7.68e+001	Ci
INVWP106	6.79e-001	Ci	INVWP106	1.33e-002	Ci
INVWP107	4.41e+001	Ci	INVWP107	2.31e-002	Ci
INVWP108	2.31e+003	Ci	INVWP108	2.70e-001	Ci
INVWP109	8.37e+002	Ci	INVWP109	3.84e+000	Ci
INVWP110	1.91e-001	Ci	INVWP110	3.73e-003	Ci
INVWP111	7.96e-001	Ci	INVWP111	1.56e-002	Ci
INVWP201	3.34e+000	Ci	INVWP201	2.59e-002	Ci
INVWP202	4.08e+002	Ci	INVWP202	7.57e-002	Ci
INVWP203	1.16e+002	Ci	INVWP203	4.98e-001	Ci
INVWP204	9.35e+001	Ci	INVWP204	5.85e-002	Ci
INVWP205	2.47e+003	Ci	INVWP205	1.10e+001	Ci
INVWP206	1.70e-001	Ci	INVWP206	3.32e-003	Ci
INVWP207	1.10e+001	Ci	INVWP207	5.79e-003	Ci
INVWP208	5.77e+002	Ci	INVWP208	6.76e-002	Ci
INVWP209	2.09e+002	Ci	INVWP209	9.59e-001	Ci
INVWP210	4.77e-002	Ci	INVWP210	9.33e-004	Ci
INVWP211	1.99e-001	Ci	INVWP211	3.89e-003	Ci
AM242M – Americium 242 metastable			BA137M – Barium 137 metastable		
HALFLIFE	4.79e+009	Seconds	HALFLIFE	1.53e+002	Seconds
INVWP101	2.84e-003	Ci	INVWP101	1.15e+004	Ci
INVWP102	2.85e+000	Ci	INVWP102	1.23e+005	Ci
INVWP103	3.83e-002	Ci	INVWP103	1.65e+005	Ci
INVWP104	1.06e-001	Ci	INVWP104	3.00e+005	Ci
INVWP105	0.00e+001	Ci	INVWP105	8.22e+004	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	5.79e-002	Ci	INVWP107	1.66e+005	Ci
INVWP108	0.00e+001	Ci	INVWP108	1.93e+005	Ci
INVWP109	4.66e+000	Ci	INVWP109	1.07e+005	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	4.21e-004	Ci	INVWP201	1.71e+003	Ci
INVWP202	4.27e-001	Ci	INVWP202	1.85e+004	Ci
INVWP203	6.37e-003	Ci	INVWP203	2.74e+004	Ci
INVWP204	1.51e-002	Ci	INVWP204	4.26e+004	Ci
INVWP205	0.00e+001	Ci	INVWP205	1.17e+004	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	1.45e-002	Ci	INVWP207	4.15e+004	Ci
INVWP208	0.00e+001	Ci	INVWP208	4.82e+004	Ci
INVWP209	1.17e+000	Ci	INVWP209	2.67e+004	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
C14 – Carbon 14			CD113M – Cadmium 113 metastable		
HALFLIFE	1.81e+011	Seconds	HALFLIFE	4.29e+008	Seconds
INVWP101	1.45e+000	Ci	INVWP101	0.00e+001	Ci
INVWP102	2.19e+000	Ci	INVWP102	2.06e+001	Ci
INVWP103	2.59e-001	Ci	INVWP103	1.33e+001	Ci
INVWP104	8.90e-004	Ci	INVWP104	1.56e+001	Ci
INVWP105	2.57e+000	Ci	INVWP105	0.00e+001	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	0.00e+001	Ci	INVWP107	0.00e+001	Ci
INVWP108	0.00e+001	Ci	INVWP108	5.88e+001	Ci
INVWP109	0.00e+001	Ci	INVWP109	3.31e+001	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	2.15e-001	Ci	INVWP201	0.00e+001	Ci
INVWP202	3.29e-001	Ci	INVWP202	3.08e+000	Ci
INVWP203	4.31e-002	Ci	INVWP203	2.21e+000	Ci
INVWP204	1.26e-004	Ci	INVWP204	2.21e+000	Ci
INVWP205	3.67e-001	Ci	INVWP205	0.00e+001	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	0.00e+001	Ci	INVWP207	0.00e+001	Ci
INVWP208	0.00e+001	Ci	INVWP208	1.47e+001	Ci
INVWP209	0.00e+001	Ci	INVWP209	8.28e+000	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci
CD113 – Cadmium 113			CE144 – Cerium 144		
HALFLIFE	2.93e+023	Seconds	HALFLIFE	2.46e+007	Seconds
INVWP101	2.57e-014	Ci	INVWP101	6.23e-007	Ci
INVWP102	0.00e+001	Ci	INVWP102	8.41e-008	Ci
INVWP103	0.00e+001	Ci	INVWP103	1.37e-001	Ci
INVWP104	0.00e+001	Ci	INVWP104	7.64e-009	Ci
INVWP105	0.00e+001	Ci	INVWP105	5.22e-006	Ci
INVWP106	0.00e+001	Ci	INVWP106	1.04e-021	Ci
INVWP107	2.00e-013	Ci	INVWP107	3.95e+004	Ci
INVWP108	0.00e+001	Ci	INVWP108	1.19e+005	Ci
INVWP109	0.00e+001	Ci	INVWP109	1.02e-002	Ci
INVWP110	0.00e+001	Ci	INVWP110	2.92e-022	Ci
INVWP111	0.00e+001	Ci	INVWP111	1.22e-021	Ci
INVWP201	3.80e-015	Ci	INVWP201	9.23e-008	Ci
INVWP202	0.00e+001	Ci	INVWP202	1.26e-008	Ci
INVWP203	0.00e+001	Ci	INVWP203	2.27e-002	Ci
INVWP204	0.00e+001	Ci	INVWP204	1.08e-009	Ci
INVWP205	0.00e+001	Ci	INVWP205	7.46e-007	Ci
INVWP206	0.00e+001	Ci	INVWP206	2.60e-022	Ci
INVWP207	5.01e-014	Ci	INVWP207	9.87e+003	Ci
INVWP208	0.00e+001	Ci	INVWP208	2.98e+004	Ci
INVWP209	0.00e+001	Ci	INVWP209	2.55e-003	Ci
INVWP210	0.00e+001	Ci	INVWP210	7.31e-023	Ci
INVWP211	0.00e+001	Ci	INVWP211	3.05e-022	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
CL36 – Chlorine 36			CM244 – Curium 244		
HALFLIFE	9.49e+012	Seconds	HALFLIFE	5.72e+008	Seconds
INVWP101	1.75e-002	Ci	INVWP101	3.34e+000	Ci
INVWP102	0.00e+001	Ci	INVWP102	5.06e+001	Ci
INVWP103	1.92e-003	Ci	INVWP103	8.40e+001	Ci
INVWP104	0.00e+001	Ci	INVWP104	3.85e+000	Ci
INVWP105	1.90e-002	Ci	INVWP105	2.18e+003	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	0.00e+001	Ci	INVWP107	4.30e+002	Ci
INVWP108	0.00e+001	Ci	INVWP108	5.00e+001	Ci
INVWP109	0.00e+001	Ci	INVWP109	1.20e+002	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	2.59e-003	Ci	INVWP201	4.95e-001	Ci
INVWP202	0.00e+001	Ci	INVWP202	7.58e+000	Ci
INVWP203	3.19e-004	Ci	INVWP203	1.40e+001	Ci
INVWP204	0.00e+001	Ci	INVWP204	5.45e-001	Ci
INVWP205	2.72e-003	Ci	INVWP205	3.12e+002	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	0.00e+001	Ci	INVWP207	1.08e+002	Ci
INVWP208	0.00e+001	Ci	INVWP208	1.25e+001	Ci
INVWP209	0.00e+001	Ci	INVWP209	2.99e+001	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci
CM243 – Curium 243			CM245 – Curium 245		
HALFLIFE	8.99e+008	Seconds	HALFLIFE	2.68e+011	Seconds
INVWP101	9.96e-003	Ci	INVWP101	1.55e-003	Ci
INVWP102	3.49e-004	Ci	INVWP102	2.00e-006	Ci
INVWP103	1.41e-002	Ci	INVWP103	2.86e-004	Ci
INVWP104	2.79e-002	Ci	INVWP104	8.69e-004	Ci
INVWP105	0.00e+001	Ci	INVWP105	0.00e+001	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	2.22e-002	Ci	INVWP107	2.69e-005	Ci
INVWP108	0.00e+001	Ci	INVWP108	0.00e+001	Ci
INVWP109	2.10e+000	Ci	INVWP109	1.38e-002	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	1.48e-003	Ci	INVWP201	2.30e-004	Ci
INVWP202	5.22e-005	Ci	INVWP202	3.00e-007	Ci
INVWP203	2.35e-003	Ci	INVWP203	4.76e-005	Ci
INVWP204	3.95e-003	Ci	INVWP204	1.23e-004	Ci
INVWP205	0.00e+001	Ci	INVWP205	0.00e+001	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	5.56e-003	Ci	INVWP207	6.71e-006	Ci
INVWP208	0.00e+001	Ci	INVWP208	0.00e+001	Ci
INVWP209	5.25e-001	Ci	INVWP209	3.45e-003	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

11. Parcel Corrosion and Source Term Models

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
CM246 – Curium 246			CO60 – Cobalt 60		
HALFLIFE	1.49e+011	Seconds	HALFLIFE	1.66e+008	Seconds
INVWP101	4.50e-004	Ci	INVWP101	0.00e+001	Ci
INVWP102	0.00e+001	Ci	INVWP102	3.88e+001	Ci
INVWP103	1.97e-005	Ci	INVWP103	0.00e+001	Ci
INVWP104	5.97e-005	Ci	INVWP104	0.00e+001	Ci
INVWP105	0.00e+001	Ci	INVWP105	0.00e+001	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	2.14e-006	Ci	INVWP107	6.79e+002	Ci
INVWP108	0.00e+001	Ci	INVWP108	1.72e+001	Ci
INVWP109	1.57e-003	Ci	INVWP109	1.21e+001	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	6.67e-005	Ci	INVWP201	0.00e+001	Ci
INVWP202	0.00e+001	Ci	INVWP202	5.81e+000	Ci
INVWP203	3.27e-006	Ci	INVWP203	0.00e+001	Ci
INVWP204	8.46e-006	Ci	INVWP204	0.00e+001	Ci
INVWP205	0.00e+001	Ci	INVWP205	0.00e+001	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	5.34e-007	Ci	INVWP207	1.70e+002	Ci
INVWP208	0.00e+001	Ci	INVWP208	4.29e+000	Ci
INVWP209	3.92e-004	Ci	INVWP209	3.02e+000	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci
CM247 – Curium 247			CS134 – Cesium 134		
HALFLIFE	4.92e+014	Seconds	HALFLIFE	6.50e+007	Seconds
INVWP101	1.34e-009	Ci	INVWP101	3.99e-002	Ci
INVWP102	0.00e+001	Ci	INVWP102	6.47e-001	Ci
INVWP103	0.00e+001	Ci	INVWP103	0.00e+001	Ci
INVWP104	0.00e+001	Ci	INVWP104	0.00e+001	Ci
INVWP105	0.00e+001	Ci	INVWP105	0.00e+001	Ci
INVWP106	0.00e+001	Ci	INVWP106	2.10e-010	Ci
INVWP107	2.64e-012	Ci	INVWP107	1.35e+003	Ci
INVWP108	0.00e+001	Ci	INVWP108	4.80e+003	Ci
INVWP109	0.00e+001	Ci	INVWP109	8.09e+001	Ci
INVWP110	0.00e+001	Ci	INVWP110	5.90e-011	Ci
INVWP111	0.00e+001	Ci	INVWP111	2.46e-010	Ci
INVWP201	1.98e-010	Ci	INVWP201	5.92e-003	Ci
INVWP202	0.00e+001	Ci	INVWP202	9.69e-002	Ci
INVWP203	0.00e+001	Ci	INVWP203	0.00e+001	Ci
INVWP204	0.00e+001	Ci	INVWP204	0.00e+001	Ci
INVWP205	0.00e+001	Ci	INVWP205	0.00e+001	Ci
INVWP206	0.00e+001	Ci	INVWP206	5.25e-011	Ci
INVWP207	6.60e-013	Ci	INVWP207	3.37e+002	Ci
INVWP208	0.00e+001	Ci	INVWP208	1.20e+003	Ci
INVWP209	0.00e+001	Ci	INVWP209	2.02e+001	Ci
INVWP210	0.00e+001	Ci	INVWP210	1.48e-011	Ci
INVWP211	0.00e+001	Ci	INVWP211	6.16e-011	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
CS135 – Cesium 135			EU152 – Europium 152		
HALFLIFE	7.25e+013	Seconds	HALFLIFE	4.20e+008	Seconds
INVWP101	9.01e-002	Ci	INVWP101	0.00e+001	Ci
INVWP102	1.05e+000	Ci	INVWP102	5.11e+000	Ci
INVWP103	3.33e-001	Ci	INVWP103	0.00e+001	Ci
INVWP104	8.38e-001	Ci	INVWP104	0.00e+001	Ci
INVWP105	5.74e-001	Ci	INVWP105	0.00e+001	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	3.98e-001	Ci	INVWP107	1.47e+001	Ci
INVWP108	1.00e+000	Ci	INVWP108	1.10e+001	Ci
INVWP109	2.53e+000	Ci	INVWP109	5.70e+000	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	1.34e-002	Ci	INVWP201	0.00e+001	Ci
INVWP202	1.57e-001	Ci	INVWP202	7.65e-001	Ci
INVWP203	5.54e-002	Ci	INVWP203	0.00e+001	Ci
INVWP204	1.19e-001	Ci	INVWP204	0.00e+001	Ci
INVWP205	8.21e-002	Ci	INVWP205	0.00e+001	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	9.94e-002	Ci	INVWP207	3.69e+000	Ci
INVWP208	2.51e-001	Ci	INVWP208	2.74e+000	Ci
INVWP209	6.32e-001	Ci	INVWP209	1.43e+000	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci
CS137 – Cesium 137			EU154 – Europium 154		
HALFLIFE	9.47e+008	Seconds	HALFLIFE	2.78e+008	Seconds
INVWP101	1.35e+004	Ci	INVWP101	0.00e+001	Ci
INVWP102	1.32e+005	Ci	INVWP102	2.29e+002	Ci
INVWP103	1.74e+005	Ci	INVWP103	0.00e+001	Ci
INVWP104	3.18e+005	Ci	INVWP104	0.00e+001	Ci
INVWP105	8.68e+004	Ci	INVWP105	0.00e+001	Ci
INVWP106	2.70e+003	Ci	INVWP106	9.52e-001	Ci
INVWP107	1.74e+005	Ci	INVWP107	2.48e+003	Ci
INVWP108	1.81e+005	Ci	INVWP108	1.34e+003	Ci
INVWP109	1.13e+005	Ci	INVWP109	1.49e+003	Ci
INVWP110	7.57e+002	Ci	INVWP110	2.68e-001	Ci
INVWP111	3.16e+003	Ci	INVWP111	1.12e+000	Ci
INVWP201	2.00e+003	Ci	INVWP201	0.00e+001	Ci
INVWP202	1.97e+004	Ci	INVWP202	3.44e+001	Ci
INVWP203	2.90e+004	Ci	INVWP203	0.00e+001	Ci
INVWP204	4.50e+004	Ci	INVWP204	0.00e+001	Ci
INVWP205	1.24e+004	Ci	INVWP205	0.00e+001	Ci
INVWP206	6.74e+002	Ci	INVWP206	2.38e-001	Ci
INVWP207	4.34e+004	Ci	INVWP207	6.20e+002	Ci
INVWP208	4.53e+004	Ci	INVWP208	3.36e+002	Ci
INVWP209	2.82e+004	Ci	INVWP209	3.74e+002	Ci
INVWP210	1.89e+002	Ci	INVWP210	6.69e-002	Ci
INVWP211	7.90e+002	Ci	INVWP211	2.79e-001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
EU155 – Europium 155			I129 – Iodine 129		
HALFLIFE	1.56e+008	Seconds	HALFLIFE	4.95e+014	Seconds
INVWP101	0.00e+001	Ci	INVWP101	1.42e-002	Ci
INVWP102	3.09e+001	Ci	INVWP102	7.80e-002	Ci
INVWP103	0.00e+001	Ci	INVWP103	6.38e-002	Ci
INVWP104	0.00e+001	Ci	INVWP104	1.78e-001	Ci
INVWP105	0.00e+001	Ci	INVWP105	5.26e-002	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	1.90e+003	Ci	INVWP107	0.00e+001	Ci
INVWP108	1.65e+003	Ci	INVWP108	6.52e-005	Ci
INVWP109	3.73e+002	Ci	INVWP109	0.00e+001	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	0.00e+001	Ci	INVWP201	2.10e-003	Ci
INVWP202	4.63e+000	Ci	INVWP202	1.17e-002	Ci
INVWP203	0.00e+001	Ci	INVWP203	1.06e-002	Ci
INVWP204	0.00e+001	Ci	INVWP204	2.52e-002	Ci
INVWP205	0.00e+001	Ci	INVWP205	7.52e-003	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	4.75e+002	Ci	INVWP207	0.00e+001	Ci
INVWP208	4.12e+002	Ci	INVWP208	1.63e-005	Ci
INVWP209	9.34e+001	Ci	INVWP209	0.00e+001	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci
FE55 – Iron 55			KR85 – Krypton 85		
HALFLIFE	8.52e+007	Seconds	HALFLIFE	3.38e+008	Seconds
INVWP101	0.00e+001	Ci	INVWP101	3.64e+002	Ci
INVWP102	2.48e-001	Ci	INVWP102	3.11e+003	Ci
INVWP103	0.00e+001	Ci	INVWP103	0.00e+001	Ci
INVWP104	0.00e+001	Ci	INVWP104	0.00e+001	Ci
INVWP105	0.00e+001	Ci	INVWP105	0.00e+001	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	0.00e+001	Ci	INVWP107	0.00e+001	Ci
INVWP108	5.64e+002	Ci	INVWP108	0.00e+001	Ci
INVWP109	1.10e+001	Ci	INVWP109	0.00e+001	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	0.00e+001	Ci	INVWP201	5.39e+001	Ci
INVWP202	3.71e-002	Ci	INVWP202	4.65e+002	Ci
INVWP203	0.00e+001	Ci	INVWP203	0.00e+001	Ci
INVWP204	0.00e+001	Ci	INVWP204	0.00e+001	Ci
INVWP205	0.00e+001	Ci	INVWP205	0.00e+001	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	0.00e+001	Ci	INVWP207	0.00e+001	Ci
INVWP208	1.41e+002	Ci	INVWP208	0.00e+001	Ci
INVWP209	2.75e+000	Ci	INVWP209	0.00e+001	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
NB93M – Niobium 93 metastable			NI59 – Nickel 59		
HALFLIFE	4.29e+008	Seconds	HALFLIFE	2.36e+012	Seconds
INVWP101	6.24e-008	Ci	INVWP101	1.22e-001	Ci
INVWP102	6.49e-001	Ci	INVWP102	4.02e-001	Ci
INVWP103	3.55e+000	Ci	INVWP103	8.72e-001	Ci
INVWP104	1.37e+001	Ci	INVWP104	0.00e+001	Ci
INVWP105	2.28e+000	Ci	INVWP105	8.64e+000	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	0.00e+001	Ci	INVWP107	9.60e-002	Ci
INVWP108	2.31e+000	Ci	INVWP108	5.44e-001	Ci
INVWP109	2.85e+000	Ci	INVWP109	1.66e+000	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	9.25e-009	Ci	INVWP201	1.80e-002	Ci
INVWP202	9.72e-002	Ci	INVWP202	6.03e-002	Ci
INVWP203	5.90e-001	Ci	INVWP203	1.45e-001	Ci
INVWP204	1.94e+000	Ci	INVWP204	0.00e+001	Ci
INVWP205	3.25e-001	Ci	INVWP205	1.23e+000	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	0.00e+001	Ci	INVWP207	2.40e-002	Ci
INVWP208	5.77e-001	Ci	INVWP208	1.36e-001	Ci
INVWP209	7.12e-001	Ci	INVWP209	4.14e-001	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci
ND144 – Neodymium 144			NI63 – Nickel 63		
HALFLIFE	6.62e+022	Seconds	HALFLIFE	3.03e+009	Seconds
INVWP101	1.27e-005	Ci	INVWP101	2.63e+000	Ci
INVWP102	0.00e+001	Ci	INVWP102	3.93e+001	Ci
INVWP103	0.00e+001	Ci	INVWP103	8.88e+001	Ci
INVWP104	0.00e+001	Ci	INVWP104	0.00e+001	Ci
INVWP105	0.00e+001	Ci	INVWP105	8.77e+002	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	1.94e-008	Ci	INVWP107	1.19e+001	Ci
INVWP108	0.00e+001	Ci	INVWP108	6.28e+001	Ci
INVWP109	0.00e+001	Ci	INVWP109	1.21e+002	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	1.88e-006	Ci	INVWP201	3.90e-001	Ci
INVWP202	0.00e+001	Ci	INVWP202	5.89e+000	Ci
INVWP203	0.00e+001	Ci	INVWP203	1.48e+001	Ci
INVWP204	0.00e+001	Ci	INVWP204	0.00e+001	Ci
INVWP205	0.00e+001	Ci	INVWP205	1.25e+002	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	4.86e-009	Ci	INVWP207	2.97e+000	Ci
INVWP208	0.00e+001	Ci	INVWP208	1.57e+001	Ci
INVWP209	0.00e+001	Ci	INVWP209	3.03e+001	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
NP237 – Neptunium 237			PB210 – Lead 210		
HALFLIFE	6.75e+013	Seconds	HALFLIFE	7.04e+008	Seconds
INVWP101	9.83e-002	Ci	INVWP101	2.89e-003	Ci
INVWP102	8.86e-001	Ci	INVWP102	1.29e-012	Ci
INVWP103	7.75e-001	Ci	INVWP103	1.11e-007	Ci
INVWP104	2.19e+000	Ci	INVWP104	2.08e-007	Ci
INVWP105	1.50e+000	Ci	INVWP105	1.04e-006	Ci
INVWP106	3.39e-001	Ci	INVWP106	0.00e+001	Ci
INVWP107	3.56e-002	Ci	INVWP107	0.00e+001	Ci
INVWP108	7.96e-001	Ci	INVWP108	0.00e+001	Ci
INVWP109	3.66e-001	Ci	INVWP109	0.00e+001	Ci
INVWP110	9.54e-002	Ci	INVWP110	0.00e+001	Ci
INVWP111	3.98e-001	Ci	INVWP111	0.00e+001	Ci
INVWP201	1.46e-002	Ci	INVWP201	4.29e-004	Ci
INVWP202	1.33e-001	Ci	INVWP202	1.93e-013	Ci
INVWP203	1.29e-001	Ci	INVWP203	1.85e-008	Ci
INVWP204	3.11e-001	Ci	INVWP204	2.94e-008	Ci
INVWP205	2.14e-001	Ci	INVWP205	1.49e-007	Ci
INVWP206	8.49e-002	Ci	INVWP206	0.00e+001	Ci
INVWP207	8.90e-003	Ci	INVWP207	0.00e+001	Ci
INVWP208	1.99e-001	Ci	INVWP208	0.00e+001	Ci
INVWP209	9.15e-002	Ci	INVWP209	0.00e+001	Ci
INVWP210	2.38e-002	Ci	INVWP210	0.00e+001	Ci
INVWP211	9.96e-002	Ci	INVWP211	0.00e+001	Ci
PA231 – Protactinium 231			PD107 – Palladium 107		
HALFLIFE	1.03e+012	Seconds	HALFLIFE	2.05e+014	Seconds
INVWP101	2.52e+000	Ci	INVWP101	5.55e-003	Ci
INVWP102	1.22e-004	Ci	INVWP102	9.44e-003	Ci
INVWP103	1.30e-004	Ci	INVWP103	5.98e-002	Ci
INVWP104	7.59e-004	Ci	INVWP104	1.25e-001	Ci
INVWP105	1.05e-004	Ci	INVWP105	1.87e-001	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	0.00e+001	Ci	INVWP107	5.89e-002	Ci
INVWP108	0.00e+001	Ci	INVWP108	1.63e-001	Ci
INVWP109	2.38e-001	Ci	INVWP109	1.71e-001	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	3.74e-001	Ci	INVWP201	8.23e-004	Ci
INVWP202	1.83e-005	Ci	INVWP202	1.41e-003	Ci
INVWP203	2.16e-005	Ci	INVWP203	9.94e-003	Ci
INVWP204	1.08e-004	Ci	INVWP204	1.77e-002	Ci
INVWP205	1.50e-005	Ci	INVWP205	2.67e-002	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	0.00e+001	Ci	INVWP207	1.47e-002	Ci
INVWP208	0.00e+001	Ci	INVWP208	4.07e-002	Ci
INVWP209	5.95e-002	Ci	INVWP209	4.28e-002	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
PM147 – Promethium 147			PU239 – Plutonium 239		
HALFLIFE	8.28e+007	Seconds	HALFLIFE	7.59e+011	Seconds
INVWP101	0.00e+001	Ci	INVWP101	1.38e+000	Ci
INVWP102	7.52e+001	Ci	INVWP102	3.60e+003	Ci
INVWP103	3.95e+003	Ci	INVWP103	9.10e+001	Ci
INVWP104	6.08e+001	Ci	INVWP104	1.80e+004	Ci
INVWP105	8.30e+001	Ci	INVWP105	1.41e+003	Ci
INVWP106	3.60e-008	Ci	INVWP106	1.75e+000	Ci
INVWP107	9.67e+004	Ci	INVWP107	5.16e+001	Ci
INVWP108	1.59e+005	Ci	INVWP108	5.64e+000	Ci
INVWP109	1.23e+003	Ci	INVWP109	2.55e+001	Ci
INVWP110	1.01e-008	Ci	INVWP110	4.92e-001	Ci
INVWP111	4.22e-008	Ci	INVWP111	2.06e+000	Ci
INVWP201	0.00e+001	Ci	INVWP201	2.04e-001	Ci
INVWP202	1.13e+001	Ci	INVWP202	5.39e+002	Ci
INVWP203	6.56e+002	Ci	INVWP203	1.51e+001	Ci
INVWP204	8.61e+000	Ci	INVWP204	2.54e+003	Ci
INVWP205	1.19e+001	Ci	INVWP205	2.02e+002	Ci
INVWP206	9.00e-009	Ci	INVWP206	4.38e-001	Ci
INVWP207	2.42e+004	Ci	INVWP207	1.29e+001	Ci
INVWP208	3.97e+004	Ci	INVWP208	1.41e+000	Ci
INVWP209	3.08e+002	Ci	INVWP209	6.37e+000	Ci
INVWP210	2.53e-009	Ci	INVWP210	1.23e-001	Ci
INVWP211	1.06e-008	Ci	INVWP211	5.14e-001	Ci
PU238 – Plutonium 238			PU240 – Plutonium 240		
HALFLIFE	2.77e+009	Seconds	HALFLIFE	2.06e+011	Seconds
INVWP101	4.45e+002	Ci	INVWP101	2.48e+000	Ci
INVWP102	1.22e+003	Ci	INVWP102	1.82e+003	Ci
INVWP103	1.65e+003	Ci	INVWP103	2.28e+001	Ci
INVWP104	3.46e+003	Ci	INVWP104	6.66e+001	Ci
INVWP105	8.58e+003	Ci	INVWP105	2.38e+001	Ci
INVWP106	2.08e+001	Ci	INVWP106	7.46e-001	Ci
INVWP107	5.93e+003	Ci	INVWP107	3.47e+001	Ci
INVWP108	3.07e+000	Ci	INVWP108	2.17e+000	Ci
INVWP109	1.30e+002	Ci	INVWP109	1.87e+001	Ci
INVWP110	5.84e+000	Ci	INVWP110	2.10e-001	Ci
INVWP111	2.44e+001	Ci	INVWP111	8.75e-001	Ci
INVWP201	6.59e+001	Ci	INVWP201	3.67e-001	Ci
INVWP202	1.83e+002	Ci	INVWP202	2.73e+002	Ci
INVWP203	2.74e+002	Ci	INVWP203	3.80e+000	Ci
INVWP204	4.90e+002	Ci	INVWP204	9.44e+000	Ci
INVWP205	1.22e+003	Ci	INVWP205	3.40e+000	Ci
INVWP206	5.19e+000	Ci	INVWP206	1.87e-001	Ci
INVWP207	1.48e+003	Ci	INVWP207	8.68e+000	Ci
INVWP208	7.68e-001	Ci	INVWP208	5.42e-001	Ci
INVWP209	3.25e+001	Ci	INVWP209	4.66e+000	Ci
INVWP210	1.46e+000	Ci	INVWP210	5.24e-002	Ci
INVWP211	6.09e+000	Ci	INVWP211	2.19e-001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
PU241 – Plutonium 241			PU244 – Plutonium 244		
HALFLIFE	4.54e+008	Seconds	HALFLIFE	2.61e+015	Seconds
INVWP101	0.00e+001	Ci	INVWP101	0.00e+001	Ci
INVWP102	3.71e+004	Ci	INVWP102	0.00e+001	Ci
INVWP103	8.01e+003	Ci	INVWP103	6.38e-009	Ci
INVWP104	3.50e+003	Ci	INVWP104	1.82e-008	Ci
INVWP105	1.34e+005	Ci	INVWP105	0.00e+001	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	6.68e+003	Ci	INVWP107	0.00e+001	Ci
INVWP108	1.03e+002	Ci	INVWP108	0.00e+001	Ci
INVWP109	1.26e+003	Ci	INVWP109	0.00e+001	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	0.00e+001	Ci	INVWP201	0.00e+001	Ci
INVWP202	5.56e+003	Ci	INVWP202	0.00e+001	Ci
INVWP203	1.33e+003	Ci	INVWP203	1.06e-009	Ci
INVWP204	4.96e+002	Ci	INVWP204	2.58e-009	Ci
INVWP205	1.92e+004	Ci	INVWP205	0.00e+001	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	1.67e+003	Ci	INVWP207	0.00e+001	Ci
INVWP208	2.58e+001	Ci	INVWP208	0.00e+001	Ci
INVWP209	3.16e+002	Ci	INVWP209	0.00e+001	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci
PU242 – Plutonium 242			RA226 – Radium 226		
HALFLIFE	1.19e+013	Seconds	HALFLIFE	5.05e+010	Seconds
INVWP101	0.00e+001	Ci	INVWP101	3.98e-005	Ci
INVWP102	6.07e-001	Ci	INVWP102	4.80e-010	Ci
INVWP103	3.28e-001	Ci	INVWP103	4.44e-007	Ci
INVWP104	1.00e-001	Ci	INVWP104	7.67e-007	Ci
INVWP105	7.93e+000	Ci	INVWP105	3.97e-006	Ci
INVWP106	3.66e-004	Ci	INVWP106	0.00e+001	Ci
INVWP107	4.89e-002	Ci	INVWP107	0.00e+001	Ci
INVWP108	5.24e-004	Ci	INVWP108	0.00e+001	Ci
INVWP109	2.54e-002	Ci	INVWP109	0.00e+001	Ci
INVWP110	1.03e-004	Ci	INVWP110	0.00e+001	Ci
INVWP111	4.29e-004	Ci	INVWP111	0.00e+001	Ci
INVWP201	0.00e+001	Ci	INVWP201	5.89e-006	Ci
INVWP202	9.10e-002	Ci	INVWP202	7.19e-011	Ci
INVWP203	5.46e-002	Ci	INVWP203	7.38e-008	Ci
INVWP204	1.42e-002	Ci	INVWP204	1.09e-007	Ci
INVWP205	1.13e+000	Ci	INVWP205	5.67e-007	Ci
INVWP206	9.14e-005	Ci	INVWP206	0.00e+001	Ci
INVWP207	1.22e-002	Ci	INVWP207	0.00e+001	Ci
INVWP208	1.31e-004	Ci	INVWP208	0.00e+001	Ci
INVWP209	6.35e-003	Ci	INVWP209	0.00e+001	Ci
INVWP210	2.57e-005	Ci	INVWP210	0.00e+001	Ci
INVWP211	1.07e-004	Ci	INVWP211	0.00e+001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
RA228 – Radium 228			RU106 – Rubidium 106		
HALFLIFE	1.82e+008	Seconds	HALFLIFE	3.18e+007	Seconds
INVWP101	4.31e-002	Ci	INVWP101	1.53e-008	Ci
INVWP102	0.00e+001	Ci	INVWP102	3.57e-005	Ci
INVWP103	0.00e+001	Ci	INVWP103	5.20e-001	Ci
INVWP104	0.00e+001	Ci	INVWP104	1.67e-007	Ci
INVWP105	0.00e+001	Ci	INVWP105	1.06e-003	Ci
INVWP106	0.00e+001	Ci	INVWP106	6.48e-019	Ci
INVWP107	0.00e+001	Ci	INVWP107	9.01e+003	Ci
INVWP108	0.00e+001	Ci	INVWP108	2.00e+004	Ci
INVWP109	2.38e-002	Ci	INVWP109	2.21e-001	Ci
INVWP110	0.00e+001	Ci	INVWP110	1.82e-019	Ci
INVWP111	0.00e+001	Ci	INVWP111	7.60e-019	Ci
INVWP201	6.39e-003	Ci	INVWP201	2.27e-009	Ci
INVWP202	0.00e+001	Ci	INVWP202	5.34e-006	Ci
INVWP203	0.00e+001	Ci	INVWP203	8.65e-002	Ci
INVWP204	0.00e+001	Ci	INVWP204	2.37e-008	Ci
INVWP205	0.00e+001	Ci	INVWP205	1.52e-004	Ci
INVWP206	0.00e+001	Ci	INVWP206	1.62e-019	Ci
INVWP207	0.00e+001	Ci	INVWP207	2.25e+003	Ci
INVWP208	0.00e+001	Ci	INVWP208	4.99e+003	Ci
INVWP209	5.95e-003	Ci	INVWP209	5.52e-002	Ci
INVWP210	0.00e+001	Ci	INVWP210	4.55e-020	Ci
INVWP211	0.00e+001	Ci	INVWP211	1.90e-019	Ci
RB87 – Rubidium 87			SB125 – Antimony 125		
HALFLIFE	1.48e+018	Seconds	HALFLIFE	8.74e+007	Seconds
INVWP101	1.13e-005	Ci	INVWP101	4.03e-002	Ci
INVWP102	4.81e-006	Ci	INVWP102	5.86e+000	Ci
INVWP103	7.08e-005	Ci	INVWP103	1.21e+002	Ci
INVWP104	2.16e-004	Ci	INVWP104	2.44e+000	Ci
INVWP105	0.00e+001	Ci	INVWP105	1.52e+001	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	3.64e-006	Ci	INVWP107	3.40e+003	Ci
INVWP108	0.00e+001	Ci	INVWP108	7.04e+003	Ci
INVWP109	0.00e+001	Ci	INVWP109	1.14e+002	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	1.67e-006	Ci	INVWP201	5.98e-003	Ci
INVWP202	7.21e-007	Ci	INVWP202	8.78e-001	Ci
INVWP203	1.18e-005	Ci	INVWP203	2.01e+001	Ci
INVWP204	3.05e-005	Ci	INVWP204	3.46e-001	Ci
INVWP205	0.00e+001	Ci	INVWP205	2.18e+000	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	9.10e-007	Ci	INVWP207	8.50e+002	Ci
INVWP208	0.00e+001	Ci	INVWP208	1.76e+003	Ci
INVWP209	0.00e+001	Ci	INVWP209	2.85e+001	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
SE79 – Selenium 79			SM151 – Samarium 151		
HALFLIFE	2.05e+012	Seconds	HALFLIFE	2.84e+009	Seconds
INVWP101	1.89e-001	Ci	INVWP101	1.09e+003	Ci
INVWP102	1.16e+000	Ci	INVWP102	2.48e+003	Ci
INVWP103	1.12e+000	Ci	INVWP103	8.69e+002	Ci
INVWP104	3.21e+000	Ci	INVWP104	2.14e+003	Ci
INVWP105	6.81e-001	Ci	INVWP105	4.77e+002	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	6.79e-001	Ci	INVWP107	9.91e+002	Ci
INVWP108	1.56e-002	Ci	INVWP108	3.34e+003	Ci
INVWP109	5.50e-002	Ci	INVWP109	1.32e+003	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	2.80e-002	Ci	INVWP201	1.61e+002	Ci
INVWP202	1.74e-001	Ci	INVWP202	3.71e+002	Ci
INVWP203	1.87e-001	Ci	INVWP203	1.44e+002	Ci
INVWP204	4.55e-001	Ci	INVWP204	3.03e+002	Ci
INVWP205	9.73e-002	Ci	INVWP205	6.81e+001	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	1.70e-001	Ci	INVWP207	2.48e+002	Ci
INVWP208	3.90e-003	Ci	INVWP208	8.36e+002	Ci
INVWP209	1.38e-002	Ci	INVWP209	3.30e+002	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci
SM147 – Samarium 147			SN121M – Tin 121 metastable		
HALFLIFE	3.34e+018	Seconds	HALFLIFE	1.73e+009	Seconds
INVWP101	4.08e-002	Ci	INVWP101	1.26e-001	Ci
INVWP102	1.76e-006	Ci	INVWP102	5.66e-001	Ci
INVWP103	1.99e-005	Ci	INVWP103	0.00e+001	Ci
INVWP104	6.07e-005	Ci	INVWP104	0.00e+001	Ci
INVWP105	0.00e+001	Ci	INVWP105	0.00e+001	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	7.99e-006	Ci	INVWP107	3.16e-001	Ci
INVWP108	0.00e+001	Ci	INVWP108	4.24e-001	Ci
INVWP109	0.00e+001	Ci	INVWP109	2.73e-001	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	6.05e-003	Ci	INVWP201	1.87e-002	Ci
INVWP202	2.64e-007	Ci	INVWP202	8.47e-002	Ci
INVWP203	3.30e-006	Ci	INVWP203	0.00e+001	Ci
INVWP204	8.60e-006	Ci	INVWP204	0.00e+001	Ci
INVWP205	0.00e+001	Ci	INVWP205	0.00e+001	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	2.00e-006	Ci	INVWP207	7.90e-002	Ci
INVWP208	0.00e+001	Ci	INVWP208	1.06e-001	Ci
INVWP209	0.00e+001	Ci	INVWP209	6.84e-002	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
SN126 – Tin 126			TC99 – Technetium 99		
HALFLIFE	3.15e+012	Seconds	HALFLIFE	6.72e+012	Seconds
INVWP101	0.00e+001	Ci	INVWP101	4.74e+000	Ci
INVWP102	2.03e+000	Ci	INVWP102	3.89e+001	Ci
INVWP103	1.08e+000	Ci	INVWP103	3.77e+001	Ci
INVWP104	2.88e+000	Ci	INVWP104	1.08e+002	Ci
INVWP105	1.35e+000	Ci	INVWP105	2.18e+001	Ci
INVWP106	0.00e+001	Ci	INVWP106	0.00e+001	Ci
INVWP107	1.77e+000	Ci	INVWP107	1.23e+001	Ci
INVWP108	1.84e+000	Ci	INVWP108	3.74e+001	Ci
INVWP109	1.63e+000	Ci	INVWP109	1.71e+000	Ci
INVWP110	0.00e+001	Ci	INVWP110	0.00e+001	Ci
INVWP111	0.00e+001	Ci	INVWP111	0.00e+001	Ci
INVWP201	0.00e+001	Ci	INVWP201	7.02e-001	Ci
INVWP202	3.03e-001	Ci	INVWP202	5.83e+000	Ci
INVWP203	1.79e-001	Ci	INVWP203	6.27e+000	Ci
INVWP204	4.07e-001	Ci	INVWP204	1.53e+001	Ci
INVWP205	1.93e-001	Ci	INVWP205	3.11e+000	Ci
INVWP206	0.00e+001	Ci	INVWP206	0.00e+001	Ci
INVWP207	4.41e-001	Ci	INVWP207	3.08e+000	Ci
INVWP208	4.60e-001	Ci	INVWP208	9.35e+000	Ci
INVWP209	4.08e-001	Ci	INVWP209	4.26e-001	Ci
INVWP210	0.00e+001	Ci	INVWP210	0.00e+001	Ci
INVWP211	0.00e+001	Ci	INVWP211	0.00e+001	Ci
SR90 – Strontium 90			TE125M – Tellurium 125 metastable		
HALFLIFE	9.19e+008	Seconds	HALFLIFE	5.01e+006	Seconds
INVWP101	1.23e+004	Ci	INVWP101	7.10e-003	Ci
INVWP102	1.03e+005	Ci	INVWP102	0.00e+001	Ci
INVWP103	1.63e+005	Ci	INVWP103	2.96e+001	Ci
INVWP104	2.97e+005	Ci	INVWP104	5.96e-001	Ci
INVWP105	5.96e+004	Ci	INVWP105	3.71e+000	Ci
INVWP106	2.31e+003	Ci	INVWP106	0.00e+001	Ci
INVWP107	1.87e+005	Ci	INVWP107	1.10e+003	Ci
INVWP108	1.67e+005	Ci	INVWP108	1.72e+003	Ci
INVWP109	1.05e+005	Ci	INVWP109	2.79e+001	Ci
INVWP110	6.50e+002	Ci	INVWP110	0.00e+001	Ci
INVWP111	2.71e+003	Ci	INVWP111	0.00e+001	Ci
INVWP201	1.83e+003	Ci	INVWP201	1.05e-003	Ci
INVWP202	1.55e+004	Ci	INVWP202	0.00e+001	Ci
INVWP203	2.71e+004	Ci	INVWP203	4.92e+000	Ci
INVWP204	4.20e+004	Ci	INVWP204	8.44e-002	Ci
INVWP205	8.52e+003	Ci	INVWP205	5.29e-001	Ci
INVWP206	5.78e+002	Ci	INVWP206	0.00e+001	Ci
INVWP207	4.67e+004	Ci	INVWP207	2.76e+002	Ci
INVWP208	4.18e+004	Ci	INVWP208	4.29e+002	Ci
INVWP209	2.62e+004	Ci	INVWP209	6.97e+000	Ci
INVWP210	1.62e+002	Ci	INVWP210	0.00e+001	Ci
INVWP211	6.78e+002	Ci	INVWP211	0.00e+001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
TH229 – Thorium 229			TH232 – Thorium 232		
HALFLIFE	2.32e+011	Seconds	HALFLIFE	4.43e+017	Seconds
INVWP101	1.85e-001	Ci	INVWP101	3.28e-002	Ci
INVWP102	3.65e-010	Ci	INVWP102	0.00e+001	Ci
INVWP103	1.44e-007	Ci	INVWP103	0.00e+001	Ci
INVWP104	1.08e-006	Ci	INVWP104	0.00e+001	Ci
INVWP105	6.99e-007	Ci	INVWP105	0.00e+001	Ci
INVWP106	0.00e+001	Ci	INVWP106	1.02e-010	Ci
INVWP107	0.00e+001	Ci	INVWP107	0.00e+001	Ci
INVWP108	0.00e+001	Ci	INVWP108	0.00e+001	Ci
INVWP109	3.29e-003	Ci	INVWP109	2.57e-002	Ci
INVWP110	0.00e+001	Ci	INVWP110	2.86e-011	Ci
INVWP111	0.00e+001	Ci	INVWP111	1.19e-010	Ci
INVWP201	2.74e-002	Ci	INVWP201	4.86e-003	Ci
INVWP202	5.47e-011	Ci	INVWP202	0.00e+001	Ci
INVWP203	2.39e-008	Ci	INVWP203	0.00e+001	Ci
INVWP204	1.53e-007	Ci	INVWP204	0.00e+001	Ci
INVWP205	9.99e-008	Ci	INVWP205	0.00e+001	Ci
INVWP206	0.00e+001	Ci	INVWP206	2.55e-011	Ci
INVWP207	0.00e+001	Ci	INVWP207	0.00e+001	Ci
INVWP208	0.00e+001	Ci	INVWP208	0.00e+001	Ci
INVWP209	8.22e-004	Ci	INVWP209	6.43e-003	Ci
INVWP210	0.00e+001	Ci	INVWP210	7.15e-012	Ci
INVWP211	0.00e+001	Ci	INVWP211	2.99e-011	Ci
TH230 – Thorium 230			U232 – Uranium 232		
HALFLIFE	2.43e+012	Seconds	HALFLIFE	2.27e+009	Seconds
INVWP101	1.33e-002	Ci	INVWP101	1.38e+001	Ci
INVWP102	6.91e-006	Ci	INVWP102	1.36e-004	Ci
INVWP103	7.14e-005	Ci	INVWP103	5.59e-003	Ci
INVWP104	1.16e-004	Ci	INVWP104	1.42e-002	Ci
INVWP105	1.59e-003	Ci	INVWP105	0.00e+001	Ci
INVWP106	3.39e-005	Ci	INVWP106	0.00e+001	Ci
INVWP107	0.00e+001	Ci	INVWP107	5.35e-002	Ci
INVWP108	0.00e+001	Ci	INVWP108	0.00e+001	Ci
INVWP109	9.41e-004	Ci	INVWP109	1.08e-001	Ci
INVWP110	9.54e-006	Ci	INVWP110	0.00e+001	Ci
INVWP111	3.98e-005	Ci	INVWP111	0.00e+001	Ci
INVWP201	1.97e-003	Ci	INVWP201	2.05e+000	Ci
INVWP202	1.04e-006	Ci	INVWP202	2.04e-005	Ci
INVWP203	1.19e-005	Ci	INVWP203	9.29e-004	Ci
INVWP204	1.65e-005	Ci	INVWP204	2.00e-003	Ci
INVWP205	2.27e-004	Ci	INVWP205	0.00e+001	Ci
INVWP206	8.49e-006	Ci	INVWP206	0.00e+001	Ci
INVWP207	0.00e+001	Ci	INVWP207	1.34e-002	Ci
INVWP208	0.00e+001	Ci	INVWP208	0.00e+001	Ci
INVWP209	2.35e-004	Ci	INVWP209	2.71e-002	Ci
INVWP210	2.39e-006	Ci	INVWP210	0.00e+001	Ci
INVWP211	9.96e-006	Ci	INVWP211	0.00e+001	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
U233 – Uranium 233			U235 – Uranium 235		
HALFLIFE	5.00e+012	Seconds	HALFLIFE	2.22e+016	Seconds
INVWP101	2.78e+001	Ci	INVWP101	1.65e-002	Ci
INVWP102	8.14e-005	Ci	INVWP102	5.57e-001	Ci
INVWP103	1.03e-004	Ci	INVWP103	2.95e-001	Ci
INVWP104	4.77e-004	Ci	INVWP104	2.00e+000	Ci
INVWP105	2.53e-004	Ci	INVWP105	7.77e-002	Ci
INVWP106	1.63e-003	Ci	INVWP106	2.46e-004	Ci
INVWP107	6.33e-006	Ci	INVWP107	6.29e-004	Ci
INVWP108	0.00e+001	Ci	INVWP108	7.88e-004	Ci
INVWP109	1.41e-001	Ci	INVWP109	1.41e-003	Ci
INVWP110	4.59e-004	Ci	INVWP110	6.91e-005	Ci
INVWP111	1.92e-003	Ci	INVWP111	2.88e-004	Ci
INVWP201	4.12e+000	Ci	INVWP201	2.45e-003	Ci
INVWP202	1.22e-005	Ci	INVWP202	8.33e-002	Ci
INVWP203	1.72e-005	Ci	INVWP203	4.91e-002	Ci
INVWP204	6.76e-005	Ci	INVWP204	2.84e-001	Ci
INVWP205	3.61e-005	Ci	INVWP205	1.11e-002	Ci
INVWP206	4.09e-004	Ci	INVWP206	6.15e-005	Ci
INVWP207	1.58e-006	Ci	INVWP207	1.57e-004	Ci
INVWP208	0.00e+001	Ci	INVWP208	1.97e-004	Ci
INVWP209	3.54e-002	Ci	INVWP209	3.53e-004	Ci
INVWP210	1.15e-004	Ci	INVWP210	1.73e-005	Ci
INVWP211	4.79e-004	Ci	INVWP211	7.21e-005	Ci
U234 – Uranium 234			U236 – Uranium 236		
HALFLIFE	7.72e+012	Seconds	HALFLIFE	7.39e+014	Seconds
INVWP101	3.54e+000	Ci	INVWP101	3.22e-001	Ci
INVWP102	1.63e+001	Ci	INVWP102	1.83e+000	Ci
INVWP103	3.27e-001	Ci	INVWP103	1.25e+000	Ci
INVWP104	5.41e-001	Ci	INVWP104	3.66e+000	Ci
INVWP105	5.89e+000	Ci	INVWP105	1.16e+000	Ci
INVWP106	4.02e-002	Ci	INVWP106	5.50e-004	Ci
INVWP107	1.37e-001	Ci	INVWP107	4.51e-003	Ci
INVWP108	1.93e-002	Ci	INVWP108	1.90e-003	Ci
INVWP109	6.58e-002	Ci	INVWP109	4.38e-003	Ci
INVWP110	1.13e-002	Ci	INVWP110	1.54e-004	Ci
INVWP111	4.71e-002	Ci	INVWP111	6.45e-004	Ci
INVWP201	5.25e-001	Ci	INVWP201	4.78e-002	Ci
INVWP202	2.44e+000	Ci	INVWP202	2.73e-001	Ci
INVWP203	5.44e-002	Ci	INVWP203	2.07e-001	Ci
INVWP204	7.67e-002	Ci	INVWP204	5.19e-001	Ci
INVWP205	8.41e-001	Ci	INVWP205	1.65e-001	Ci
INVWP206	1.00e-002	Ci	INVWP206	1.37e-004	Ci
INVWP207	3.43e-002	Ci	INVWP207	1.13e-003	Ci
INVWP208	4.82e-003	Ci	INVWP208	4.75e-004	Ci
INVWP209	1.64e-002	Ci	INVWP209	1.10e-003	Ci
INVWP210	2.82e-003	Ci	INVWP210	3.86e-005	Ci
INVWP211	1.18e-002	Ci	INVWP211	1.61e-004	Ci

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

Table 11-9. Modeling Parameters for the Radionuclides (Continued)

Parameter*	Value	Units	Parameter*	Value	Units
U238 – Uranium 238			ZR93 – Zirconium 93		
HALFLIFE	1.41e+017	Seconds	HALFLIFE	4.82e+013	Seconds
INVWP101	3.80e-004	Ci	INVWP101	7.50e+000	Ci
INVWP102	1.18e+001	Ci	INVWP102	5.46e+000	Ci
INVWP103	5.87e-002	Ci	INVWP103	5.73e+000	Ci
INVWP104	2.16e-001	Ci	INVWP104	1.65e+001	Ci
INVWP105	1.43e+000	Ci	INVWP105	3.01e+000	Ci
INVWP106	1.38e-005	Ci	INVWP106	0.00e+001	Ci
INVWP107	4.20e-002	Ci	INVWP107	4.47e+000	Ci
INVWP108	1.49e-002	Ci	INVWP108	5.16e+000	Ci
INVWP109	1.25e-002	Ci	INVWP109	4.27e+000	Ci
INVWP110	3.88e-006	Ci	INVWP110	0.00e+001	Ci
INVWP111	1.62e-005	Ci	INVWP111	0.00e+001	Ci
INVWP201	5.64e-005	Ci	INVWP201	1.11e+000	Ci
INVWP202	1.77e+000	Ci	INVWP202	8.18e-001	Ci
INVWP203	9.76e-003	Ci	INVWP203	9.53e-001	Ci
INVWP204	3.06e-002	Ci	INVWP204	2.34e+000	Ci
INVWP205	2.05e-001	Ci	INVWP205	4.29e-001	Ci
INVWP206	3.45e-006	Ci	INVWP206	0.00e+001	Ci
INVWP207	1.05e-002	Ci	INVWP207	1.12e+000	Ci
INVWP208	3.72e-003	Ci	INVWP208	1.29e+000	Ci
INVWP209	3.13e-003	Ci	INVWP209	1.07e+000	Ci
INVWP210	9.69e-007	Ci	INVWP210	0.00e+001	Ci
INVWP211	4.05e-006	Ci	INVWP211	0.00e+001	Ci
Y90 – Yttrium 90					
HALFLIFE	2.30e+005	Seconds			
INVWP101	1.23e+004	Ci			
INVWP102	1.03e+005	Ci			
INVWP103	1.63e+005	Ci			
INVWP104	2.97e+005	Ci			
INVWP105	5.96e+004	Ci			
INVWP106	2.31e+003	Ci			
INVWP107	1.91e+005	Ci			
INVWP108	1.67e+005	Ci			
INVWP109	1.05e+005	Ci			
INVWP110	6.50e+002	Ci			
INVWP111	2.71e+003	Ci			
INVWP201	1.83e+003	Ci			
INVWP202	1.55e+004	Ci			
INVWP203	2.71e+004	Ci			
INVWP204	4.20e+004	Ci			
INVWP205	8.52e+003	Ci			
INVWP206	5.78e+002	Ci			
INVWP207	4.79e+004	Ci			
INVWP208	4.18e+004	Ci			
INVWP209	2.62e+004	Ci			
INVWP210	1.62e+002	Ci			
INVWP211	6.78e+002	Ci			

* INVWP equals the inventory per waste parcel e.g., for waste parcel 101.

12. Complex Consequence Modeling

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The computationally intensive performance assessment, the "Complex PA," is designed to study the movement of radioactive waste by means of a series of flow and transport numerical models in a Monte Carlo analysis. The principal models used are shown in Table 12-1 and described in this chapter. Other important models and submodels used in the Complex PA are GASSNF and CONRAD. GASSNF is described in Chapter 11, and CONRAD is described in Section 12.2.

Table 12-1. Flow and Transport Models for the Complex PA

Model	Description	Section
BRAGFLO_T	Unsaturated thermal hydraulics	12.1
NUTS	Unsaturated transport	12.3
STAFF3D	Saturated flow and transport	12.4

In a Monte Carlo analysis, parameter uncertainty and sensitivity to the solution are investigated by performing a number of simulations with different sets of input parameters. In this analysis, 38 simulations were performed for each of two repository designs (vertical and horizontal waste emplacement). The 38 simulations consist of 36 sampling realizations, plus two parameter sets that contain only mean or median value parameters.

12.1 Repository Fluid Flow and Temperature Modeling

12.1.1 Mathematical Model Description

BRAGFLO_T (ver. 2.00) is the numerical simulator used to compute the flow of water, air, and heat, in the Complex PA. BRAGFLO_T is an enhanced version of the isothermal multiphase flow model, BRAGFLO (WIPP PA, 1992b, Vol. 2, Appendix A). The enhancements include the addition of the energy balance equation and the incorporation of thermal effects on both fluid and rock properties. The code also contains submodels that predict gas and water consumption/production as the result of waste package corrosion, and a submodel that predicts the energy released as the result of radioactive decay of the waste. Version 2.00 includes many features and solution techniques used in TOUGH2 (Pruess, 1991), such as an effective continuum approximation for modeling fractured porous media, vapor pressure lowering due to capillary pressure, and diffusive mass flux in the gas phase.

The code uses a finite-difference formulation to solve three partial differential equations (PDEs) that describe the mass and energy balance of a two-component, two-phase system. Fick's Law and a multiphase extension of Darcy's Law are used to describe fluid flow. Heat is transported by conduction and convection, the latter including both sensible and latent heat. The following are the governing partial differential equations solved by BRAGFLO_T:

Component mass balance equations ($i = 1, 2$):

$$\nabla \cdot \left[\frac{\alpha y_i \rho_n k_{rn} k}{\mu_n} (\nabla P_n + \rho_n g \nabla Z) + \frac{\alpha x_i \rho_w k_{rw} k}{\mu_w} (\nabla P_w + \rho_w g \nabla Z) + \frac{\alpha \rho_n \phi S_n D_{ij}}{\tau} \nabla y_i \right] + \alpha \left[y_i^s q_n^s + x_i^s q_w^s + y_i^c q_n^c + x_i^c q_w^c \right] = \alpha \frac{\partial}{\partial t} [y_i \phi \rho_n S_n + x_i \phi \rho_w S_w] \quad (12.1-1)$$

Energy balance equation:

$$\begin{aligned} \nabla \cdot (\alpha \lambda \nabla T) + \nabla \cdot \left[\frac{\alpha h_n \rho_n k_{rn} k}{\mu_n} (\nabla P_n + \rho_n g \nabla Z) + \frac{\alpha h_w \rho_w k_{rw} k}{\mu_w} (\nabla P_w + \rho_w g \nabla Z) \right] \\ + \alpha [h_n^s q_n^s + h_w^s q_w^s + h_n^c q_n^c + h_w^c q_w^c] = \alpha \frac{\partial}{\partial t} [\phi (U_n \rho_n S_n + U_w \rho_w S_w) + (1 - \phi) \rho_r U_r] \end{aligned} \quad (12.1-2)$$

where

- x_i = mass fraction of component i in the wetting phase [dimensionless]
- y_i = mass fraction of component i in the nonwetting phase [dimensionless]
- ρ = density [kg/m³]
- μ = dynamic viscosity [N·s/m²]
- k = permeability [m²]
- k_r = relative permeability [dimensionless]
- P = pressure [Pa]
- S = saturation [dimensionless]
- ϕ = porosity [dimensionless]
- h = enthalpy [J/kg]
- U = internal energy [J/kg]
- D_{ij} = gas diffusion coefficient of component i in a mixture of i and j [m²/s]
- τ = tortuosity [dimensionless]
- t = time [s]
- g = gravitational acceleration [m/s²]
- Z = elevation [m]
- q = source/sink term [kg/(m³·s)]
- α = dimension-dependent geometry term [(1D = $\Delta y \Delta z$, m²), (2D = Δz , m), (3D = 1, dimensionless)]

In Equation 12.1-1, the mass balance is compositional with respect to component i , where i is equal to 1 for the noncondensable component (air), and 2 for the condensable component (water). Subscripts w and n refer to the wetting and nonwetting phases, respectively, while subscript r refers to the rock. Superscripts are used to distinguish the origin of a source/sink term; s refers to wells, and c to chemical reactions.

Complex numerical models, such as BRAGFLO_T (2.00), are typically verified by comparing the results of the simulator with both analytical solutions and similar numerical models. BRAGFLO_T (2.00) was verified using an analytical solution to the heat pipe problem (Udell and Fitch, 1985) and TOUGH (Pruess et al., 1990), a comparable numerical simulator. Verification results are presented in Appendix G.

Effective Continuum. To simulate the thermohydrologic processes of a fractured porous medium, an effective continuum approximation (Pruess et al., 1990; Peters and Klaveter, 1988) was added to BRAGFLO_T. The model is based on the assumption that a state of local thermodynamic equilibrium (phase pressures and temperatures) exists between the matrix and fracture network. This assumption greatly simplifies the mathematical description of a fractured porous medium by cutting the number of unknowns in half. Consequently, the fractured porous medium can be represented by a single effective continuum with one set of thermodynamic variables describing the state of the system.

Peters and Klaveter (1988) present a detailed discussion of the mathematical simplifications needed to derive the effective continuum formulation for Richards equation (Richards, 1931). Pruess et al. (1990) extended the work to multiphase flow. The effective continuum implemented in BRAGFLO_T is very similar to that of Pruess et al. (1990); however, there are slight differences, warranting a brief description of the formulation used. A technique is also presented to extract the matrix and fracture flow fields from the effective continuum solution. Decoupling the effective continuum solution is necessary to perform the dual-permeability radionuclide transport calculations discussed in Section 12.3.

To implement the effective continuum model, parameters and characteristic curves representative of the fractured porous medium must be obtained. These parameters and expressions are derived from the properties of the rock matrix and the interconnected fractures. Designating matrix parameters with the subscript m, and fracture parameters with the subscript f, the total volume of the system, V, is

$$V = V_m + V_f \quad (12.1-3)$$

The effective matrix porosity, $\bar{\phi}_m$ (matrix pore volume divided by the total volume), is calculated from the matrix porosity, ϕ_m (matrix pore volume divided by the matrix volume).

$$\bar{\phi}_m = \phi_m \frac{V_m}{V} \quad (12.1-4)$$

Similarly, the effective fracture porosity, $\bar{\phi}_f$, is computed as,

$$\bar{\phi}_f = \phi_f \frac{V_f}{V} \quad (12.1-5)$$

The effective total porosity, ϕ , defined as the total pore volume divided by the total volume, is then the sum of the effective matrix and effective fracture porosities.

$$\phi = \bar{\phi}_m + \bar{\phi}_f \quad (12.1-6)$$

The effective continuum wetting phase saturation, S_w , is computed in a like manner in terms of the wetting phase matrix and fracture saturations, $S_{w,m}$ and $S_{w,f}$.

$$S_w = \frac{S_{w,m}\phi_m V_m + S_{w,f}\phi_f V_f}{\phi_m V_m + \phi_f V_f} \quad (12.1-7)$$

The matrix and fracture network can be conceptualized as a parallel flow system in each of the principle coordinate directions. Thus, the effective continuum absolute permeability is calculated in each coordinate direction, and is expressed in terms of the matrix and fracture permeabilities, k_m and k_f and the cross-sectional areas of each, A_m and A_f (Amyx et al., 1960).

$$k = \frac{A_m k_m + A_f k_f}{A_m + A_f} \quad (12.1-8)$$

Including the relative permeability of the matrix and the fracture, $k_{r,m}$ and $k_{r,f}$, an analogous averaging formula describes the effective permeability to the phase β , $k_{e\beta}$ (β = wetting, or nonwetting phase),

$$k_{e\beta} = \frac{A_m k_{r\beta,m} k_m + A_f k_{r\beta,f} k_f}{A_m + A_f} \quad (12.1-9)$$

The effective continuum relative permeability to phase β , $k_{r\beta}$, is derived from Equations 12.1-8 and 12.1-9,

$$k_{r\beta} = \frac{k_{e\beta}}{k} = \frac{A_m k_{r\beta,m} k_m + A_f k_{r\beta,f} k_f}{A_m k_m + A_f k_f} \quad (12.1-10)$$

The effective continuum relative permeability is a function of the relative permeabilities in the matrix and the fracture, which are functions of their respective wetting phase saturations. Therefore, to evaluate Equation 12.1-10, the wetting phase saturation in the matrix and the fracture must be obtained. This is accomplished by imposing the assumption of local thermodynamic equilibrium, which establishes the constraint that,

$$P_{c,m}(S_{w,m}) = P_{c,f}(S_{w,f}) \quad (12.1-11)$$

The matrix and fracture wetting phase saturations are then computed by simultaneously solving Equations 12.1-7 and 12.1-11.

Matrix and Fracture Darcy Velocities. Upon solving the mass and energy balance equations, the phase pressures, saturations, and temperatures are known at specified times and locations. Darcy's law, extended to multiphase, is then used to compute the total mass flux rate between adjacent grid block centers. In an upstream weighted, block centered, finite difference formulation, the discretized form of Darcy's law (Aziz and Settari, 1979) is written as

$$Q_{T_{i-1/2}} = -\left(k_{r\beta}\right)_{up} \left(\frac{kA\rho_{\beta}}{\mu_{\beta}}\right)_{i-1/2} \left[\frac{P_i^* - P_{i-1}^*}{1/2(\Delta x_i + \Delta x_{i-1})}\right], \quad (12.1-12)$$

where, Q_T is the mass flux in the x direction of the phase between grid blocks located at i and $i-1$, and P^* is the pressure head

$$P^* = P + \rho gh. \quad (12.1-13)$$

The total mass flux is simply the sum of the matrix mass flux, Q_m , and the fracture mass flux, Q_f

$$Q_{T_{i-1/2}} = Q_{m_{i-1/2}} + Q_{f_{i-1/2}}. \quad (12.1-14)$$

To estimate Q_m and Q_f Equation 12.1-12 is partitioned into a matrix and fracture component as in Equation 12.1-14. This partition is accomplished by first substituting Equations 12.1-9 and 12.1-10 into Equation 12.1-12 ($A = A_m + A_f$),

$$Q_{T_{i-1/2}} = \left(\frac{A_m k_{r\beta,m} k_m + A_f k_{r\beta,f} k_f}{kA}\right)_{up} \left(\frac{kA\rho_{\beta}}{\mu_{\beta}}\right)_{i-1/2} \left[\frac{P_i^* - P_{i-1}^*}{1/2(\Delta x_i + \Delta x_{i-1})}\right] \quad (12.1-15)$$

If it were possible to remove the product " kA " from the denominator of the first term and the numerator of the second term, the equation would reduce to the sum of Darcy's law written for each continuum. However, because the first term (relative permeability) is evaluated at the upstream grid block and the second term (interblock flow) is evaluated at the interface between grid blocks i and $i-1$, the product " kA " does not drop out of the equation. We can, however, "estimate" Q_m and Q_f by distributing the mass flux proportionally based on the contribution each continuum makes to the effective relative permeability,

$$Q_{m_{i-1/2}} = -\left(\frac{A_m k_{r\beta,m} k_m}{kA}\right)_{up} \left(\frac{kA\rho_{\beta}}{\mu_{\beta}}\right)_{i-1/2} \left[\frac{P_i^* - P_{i-1}^*}{1/2(\Delta x_i + \Delta x_{i-1})}\right] \quad (12.1-16)$$

$$Q_{f_{i-1/2}} = -\left(\frac{A_f k_{r\beta,f} k_f}{kA}\right)_{up} \left(\frac{kA\rho_{\beta}}{\mu_{\beta}}\right)_{i-1/2} \left[\frac{P_i^* - P_{i-1}^*}{1/2(\Delta x_i + \Delta x_{i-1})}\right]. \quad (12.1-17)$$

This formulation is consistent with Equations 12.1-12 and 12.1-14, and reduces to Darcy's law when the product " kA " of the upstream grid block is equal to " kA " at the grid block interface.

Boundary Heat Loss. Heat is transported across specified problem domain boundaries using a one-dimensional analytical solution to the heat equation,

$$\frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} \quad (12.1-18)$$

where

k = thermal diffusivity [m^2/s]
 T = temperature [K]
 t = time [s]
 x = distance [m].

The boundary condition is

$T(0, t) = F(t), t \geq 0$ (given temperature history),

and initial condition is

$T(x, 0) = T_1, x \geq 0$ (given initial temperature).

The diffusivity is expressed in terms of the formation properties as

$$k = K/\rho c \quad (12.1-19)$$

where

K = thermal conductivity [J/s/m/K]
 ρ = density [kg/m^3]
 c = specific heat [J/kg/K]

Let

t_i = i th time in simulation, $i = 1, \dots, n + 1$
 T_i = temperature at i th time
 $\Delta T_i = T_{i+1} - T_i$ (temperature increment over i th time step).

Note T_1 is temperature at initial time t_1 .

The solution of Equation 12.3-1 with the above initial and boundary conditions was derived by Carslaw and Jaeger (1959). The result of their work is

$$T - T_1 = \sum_{i=1}^n \Delta T_i \operatorname{erfc} \left[\frac{x}{2\sqrt{k(t-t_i)}} \right] \quad (12.1-20)$$

where erfc is the complementary error function. The temperature gradient at the boundary $x = 0$ is computed to be

$$\frac{\partial T}{\partial x}(0, t) = -\frac{1}{\sqrt{\pi k}} \sum_{i=1}^n \Delta T_i / \sqrt{t-t_i}, \quad t_n \leq t \leq t_{n+1} \quad (12.1-21)$$

The cumulative heat flux over the time step is obtained from

$$Q_{\text{boundary}} = -\int_{t_n}^{t_{n+1}} KA \frac{\partial T}{\partial x}(0, t) dt \quad (12.1-22)$$

and is found to be

$$Q_{\text{boundary}} = E(n) - E(n-1) \quad (12.1-23)$$

where

$$E(n) = \frac{2KA}{\sqrt{\pi k}} \sum_{i=1}^n \Delta T_i \sqrt{t_{n+1} - t_i} \quad (12.1-24)$$

Capillary Pressure. At the boundary between two phases, an imbalance in molecular forces creates a component of force acting tangential to the interface between the two phases, referred to as the interfacial tension. Interfacial tension acting on a curved surface is balanced, at equilibrium, by pressure differences between the two phases. The difference in pressure is called the capillary pressure, P_c , and is defined as,

$$P_c = P_w - P_n$$

Though capillary effects dominate P_c at high to moderately low wetting phase saturations, wetting phase adsorption to the solid phase dominates P_c at low saturations (Melrose, 1991). To model both the capillary and phase adsorption effects, two mathematical expressions were selected; the van Genuchten (1980) model and the Ross et al. (1992) exponential model. In a manner very similar to that proposed by Rossi and Nimmo (1994), the two mathematical models were combined in a piecewise fashion, as follows:

$$S_w < S_{wj} \quad P_{c1} = P_m \exp\left(\frac{-S_w}{C}\right) \quad (12.1-25)$$

$$S_w < S_{wj} \quad P_{c2} = P_o \left(S_e^{[n/(1-n)]} - 1 \right)^{1/n} \quad (12.1-26)$$

The exponential model, Equation 12.1-25, describes phase adsorption effects at low wetting phase saturations. The parameters, P_m and C , are constants, where P_m is the maximum possible capillary pressure at zero wetting phase saturation. The exponential model is joined to the van Genuchten model, Equation 12.1-26, at the junction saturation, S_{wj} . The parameters P_o and n , are constants dependent on the rock type. S_e is the "effective" wetting phase saturation defined by,

$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr}} \quad (12.1-27)$$

where, S_{wr} , is the residual wetting phase saturation. Luckner et al. (1989) define S_{wr} as the point "when all or parts of the connecting films become so thin, and hence so strongly adsorbed onto the solid phase, that the wetting fluid loses its capability to respond to hydraulic gradients." Therefore, S_{wj} is always greater than S_{wr} , but only by a small margin.

Making the piecewise function both continuous and smooth at S_{wj} , the following constraints are imposed;

$$P_{c1}(S_{wj}) = P_{c2}(S_{wj}) \quad (12.1-28)$$

$$\frac{\partial}{\partial S_w} P_{c1}(S_{wj}) = \frac{\partial}{\partial S_w} P_{c2}(S_{wj}) \quad (12.1-29)$$

Distributions of the van Genuchten parameters P_o and n , are known from the extensive research already conducted at Yucca Mountain. P_m is assumed to be constant and formation independent as suggested by Rossi and Nimmo (1994). The remaining unknowns, C and S_{wj} , are found by solving the nonlinear Equations 12.1-41 and 12.1-42 simultaneously.

During the solution process, it was necessary to use a value of 10^{11} Pa for P_m to ensure that a value of C and S_{wj} could be solved that satisfied the conditions in Equations 12.1-41 and 12.1-42 for all sample sets. Although this value is somewhat higher than that suggested by Rossi and Nimmo (1994), 1×10^9 to 5×10^9 Pa, the quantitative value of

P_m is considerably uncertain. Furthermore, the influence of this parameter on the overall solution is thought to be minimal.

The most important benefit of the piecewise capillary pressure model is that it allows water/vapor phase changes to take place at, above, and below S_{wr} . The original van Genuchten model cannot handle conditions of $S_w \leq S_{wr}$. This difference is shown graphically in Figure 12-1, where the van Genuchten and the piecewise model are plotted using median parameter values of the TSw matrix (Table 12-2).

TRI-6342-5044-0

Figure 12-1. Comparison of van Genuchten and piecewise models.

Table 12-2. TSw Median Capillary Pressure and Relative Permeability Parameters

	Matrix	Fracture
n	1.62	3.0
P_o (Pa)	8.806×10^5	1246×10^3
S_{wr}	0.02124	0.04
S_{nr}	0.02124	0.04
S_{wj}	0.03320	0.04139
P_m (Pa)	1×10^{11}	1×10^{11}
C	7.379×10^{-3}	2.772×10^{-3}

The median value capillary pressure functions for both the matrix and the fracture in the TSw are plotted in Figure 12-2. Notice that the capillary pressure of the matrix greatly exceeds the capillary pressure of the fracture over most of the diagram. Furthermore, the assumption of local equilibrium imposed as part of the effective continuum approximation inherently implies capillary pressure equilibrium between the matrix and the fracture. A primary limitation of this work is that in order to activate fracture flow, $S_w > S_{wr}$, the matrix must first be highly water saturated. Therefore, the possibility of water preferentially flowing through the fracture network in unsaturated rock (i.e., the WEEPS model) is not modeled in the Complex PA.

TRI-6342-5045-0

Figure 12-2. Median value capillary pressure functions for both matrix and fracture in TSw.

Relative Permeability. The relative permeability functions used in this study were presented by Luckner et al. (1989) and based on the theory of Mualem (1976). They are;

$$k_{rw} = S_e^{1/2} \left[1 - (1 - S_e^{1/m})^m \right]^2 \quad (12.1-30)$$

$$k_{rn} = (S_e^*)^{1/3} \left[1 - (1 - S_e^*)^{1/m} \right]^{2m} \quad (12.1-31)$$

where, k_{rw} and k_{rn} are the wetting and nonwetting phase relative permeabilities, respectively, m is derived from the van Genuchten parameter n , $m = 1 - 1/n$, and S_e^* is the nonwetting phase effective saturation,

$$S_e^* = \frac{S_n - S_{nr}}{1 - S_{nr}} \quad (12.1-32)$$

S_n is the nonwetting phase saturation, and S_{nr} is the nonwetting phase residual saturation. Median value wetting and nonwetting relative permeability functions of the TSw matrix are shown in Figure 12-3.

12.1.2 Applied Model

Model Geometry and Spatial Discretization. In the unsaturated zone, fluid and heat flow are modeled in two dimensions using the computational meshes depicted in Figure 12-4 (horizontal waste emplacement), and Figure 12-5 (vertical waste emplacement). These diagrams are essentially a vertical cross-section through the repository and surrounding geologic strata. Each square represents a grid block in the finite difference spatial discretization. Integers on the drawings (shown in reverse type) represent the two-dimensional element indices. The grid blocks, as shown, are not to scale. Instead, each cell is displayed with unit dimensions. The actual grid block dimensions are shown below the grid for the x-direction, above the grid for the y-direction, and to the left of the grid for the z-direction.

TRI-6342-5046-0

Figure 12-3. Median value wetting and nonwetting relative permeability functions of the TSw matrix.

Fluid and energy transport are modeled from the surface to the water table. Both computation meshes are based on the stratigraphic column of Yucca Mountain, shown in Chapter 5 (Figure 5-6). All geologic units are assumed to be homogenous and of constant thickness. The mesh extends horizontally 5 km beyond the edge of the repository, and a 2.4-km regulatory boundary is embedded in the mesh.

All geologic layering is assumed to be horizontal. Though obviously in error, this assumption was necessary to eliminate numerical instability problems associated with grid blocks that pass through the water table. The instability is caused by the highly nonlinear behavior of the wetting phase, effective continuum, relative permeability curve as the liquid saturation approaches 100%. Interaction of the water table with the unsaturated zone is included, but the water table is held at a constant elevation of 730 m, positioning it near the bottom of the Calico Hills nonwelded zeolitic member (CHnz).

By neglecting the effects of formation dip, the problem becomes axisymmetric about the center of the repository. Consequently, only half the repository and geologic barrier are modeled; the other half is the mirror image. An artistic view of the axis of symmetry and the spacial discretization, as seen from above, is presented in Figure 12-6. Notice that rectangular elements are used within the repository, and radial elements are used in the surrounding rock. Use of the two element types creates a transitional region (shaded area in Figure 12-6).

The top view can be approximated in one dimension, as shown in Figure 12-7. Here the transitional region is represented by two elements and placed adjacent to the repository. The combined length of the transitional elements, x , is taken as, $r - L/2$, and the thickness is computed to conserve volume. Next to the transitional elements are the radial elements. The thickness of the radial elements increases as the distance from the repository increases, again to conserve volume. This combination of rectangular and axisymmetric modeling has been used previously by the WIPP PA Department to model fluid flow in a system that is not fully axisymmetric (Rechard et al., 1990, p. 37; Rechard et al., 1993, p. 12-12).

The repository floor is located at an elevation of 1033 m in both the horizontal and vertical emplacement designs. In the horizontal design, the waste packages are disposed of in a horizontal orientation inside the disposal rooms. Each room holds 74.3 multi-purpose canisters (MPCs). The horizontal emplacement repository contains 59 disposal

12. Complex Consequence Modeling

- Average Water Infiltration
- Repository Water Infiltration
- ▲ Enhanced Water Infiltration
- × Constant Water Pressure

Figure 12-4. Horizontal Waste Emplacement Computational Mesh.

Figure 12-5. Vertical Waste Emplacement Computational Mesh.

TRI-6342-5063-0

Figure 12-6. Horizontal spatial discretization in two dimensions.

TRI-6342-5043-0

Figure 12-7. Horizontal spatial discretization in one dimension.

rooms, 4.30 m in diameter, spaced 4.30 m apart. Because only half the repository is modeled, 29.5 disposal rooms are included. The first grid block in the waste region contains 1-1/2 disposal rooms, 1-1/2 pillars, and a portion of the front and back accessways, for a total length of 12.9 m (Figure 12-8). The next 28 grid blocks are 8.6 m in length and contain one disposal room and one pillar each. The last grid block, shaded in Figure 12-4, contains the accessway at the end of the repository and one-half of the last pillar. All repository grid blocks are of constant thickness, equal to the width of the repository, 456.36 m.

In the vertical emplacement design, the waste packages are disposed of in circular holes drilled beneath the repository floor (Section 6.3). Each grid block in the waste region contains the waste of a single disposal room, 490.7 waste packages. Each grid block above the repository floor contains one disposal room, one pillar separating the rooms, and a portion of the front and back accessways (Figure 12-9). The repository contains a total of 38 disposal rooms, 7.62 m in diameter, spaced 7.50 m apart. Once again, only half the repository is modeled, leaving 19 disposal rooms. Thus, 19 grid blocks, each 15.12 m in length, represent the vertical emplacement repository. As in the horizontal emplacement design, the last grid block in the drift region, shaded in Figure 12-5, contains the accessway at the end of the repository and one-half of the last pillar.

From a thermal hydraulic perspective, the main difference between the vertical and horizontal waste emplacement repositories is the thermal loading. The total length of the horizontal emplacement repository, including accessways, is 526.9 m. The total length of the vertical emplacement repository is 597.3 m. Both repositories are the same width. Therefore, the horizontal emplacement repository is slightly smaller than the vertical emplacement repository. Because both repositories contain the same amount of waste, the thermal loading is greater on an areal basis in the horizontal emplacement design.

TRI-6342-4295-2

Figure 12-8. Horizontal waste emplacement repository gridding.

12. Complex Consequence Modeling

TRI-6342-4295-1

Figure 12-9. Vertical waste emplacement repository gridding.

Grid blocks within the repository include waste, tuff, and void space. To simulate the thermal hydrologic behavior of these components in a single element, volumetrically averaged properties are used. As discussed in Section 12.1.1, an effective continuum approximation consisting of a two component, matrix/fracture system is used to simulate the geologic barrier. The same approach could be extended to a three- or, in this case, a four-component system. However, decoupling the flow field for the radionuclide transport calculations would then be extremely difficult, so a two-component system is maintained. To account for the void space between the waste packages and the rock matrix, this volume is incorporated into the fracture continuum by increasing the fracture porosity. The volume occupied by the waste packages is included in the matrix continuum and simply modeled as tuff matrix.

Initial Conditions. The initial thermodynamic state of the system can be defined by the initial temperature, and initial fluid phase pressures. The effects of thermal gradients are considered negligible, so the initial temperature was set equal to the repository temperature, 299.15 K (26°C), at all locations. Below the water table, the initial water pressure is calculated assuming hydrostatic equilibrium. Above the water table, the initial gas pressure is assumed to

be atmospheric, 10^5 Pa. Water pressure in the unsaturated zone is interpolated from point values. The point values are computed from sampled matrix capillary pressure parameters and the initial water saturation values given in Table 12-3. The values in Table 12-3 were obtained from the Yucca Mountain Project Reference Information Base (Version 4) and are used for each sample set. The water pressure, P_w , is calculated from the relationship,

$$P_w = P_g - P_c(S_w) \quad (12.2-1)$$

where, P_g is the initial gas pressure, and $P_c(S_w)$ is the capillary pressure.

Table 12-3. Initial Water Saturation

Geologic Member	Elevation (m)	Water Saturation
TCw	1328	0.67
PTn	1217	0.61
TSw	1033	0.65
TSv	863	0.95
CHnz	730	1.00

This approach can result in water pressure profiles that are severely out of equilibrium and unrealistic. To compensate for this possibility, each simulation is run 1000 yr before inserting the waste. The 1000-yr period permits the initial pressures and saturations to approach steady-state conditions in each parameter sample set.

Boundary Conditions. BRAGFLO_T assumes "no flow" (Neuman type with a flux rate of zero) boundary conditions for both mass and energy. Dirichlet (constant head) and Neuman (specified flux) boundary conditions can be imposed on the mass balance, though, by using constant pressure and specified flux wells in elements adjacent to the boundary. Neuman boundary conditions can be imposed on the energy balance using the boundary heat loss equation discussed in Section 12.1.

Dirichlet boundary conditions are used at the base of the CHnv to maintain the water table in a relatively stable position. This boundary condition prevents unrealistic increases in the water table elevation caused by the accumulation of infiltrating water. A constant head boundary condition is also used in the top of the TCw in the gas phase. Gas pressure is maintained at 10^5 Pa to simulate a constant atmospheric pressure condition at the surface.

Surface water infiltration is handled in the top of the TCw using specified flux water injection wells, or Neuman boundary conditions. The injection rate is a function of time computed by Equation 5-1. The parameters of the infiltration equation are sampled on, so each sample set has a different injection rate. The value computed by Equation 5-1 represents the average "regional" infiltration rate and is used in all injection wells not located directly above the repository. Circular symbols show the location of these wells in Figures 12-4 and 12-5. Above the repository, the surface infiltration rate is nonuniform. A single well (solid triangle) injects water at a rate 1 to 10 times (sample parameter) the average injection rate, simulating a rainfall catchment or any other mechanism of "locally" enhancing the surface infiltration. The injection rate of the remaining wells above the repository (square symbols) is slightly less than the average rate, computed such that the total infiltration rate above the repository is equal to the average "regional" rate.

Heat is permitted to flow across problem domain boundaries using Equation 12.1-23, in the boundary heat loss routine. This technique is used to transport heat on the right, top, and bottom mesh boundaries in Figures 12-4 and 12-5. Heat is also permitted to flow from the repository region (x indices 1-30 for horizontal emplacement and 1-20 for vertical emplacement) in the y-direction (into and out of the page), as shown in Figure 12-7. Use of the boundary heat loss routine in the y-direction allows heat to flow in all three dimensions from the repository. The three-dimensional representation should produce good results particularly in the center of the repository.

Input Data. For all modeling parameters that were not sampled, the median value of that parameter is used in all 36 sample sets. However, at the time the BRAGFLO_T computations were performed, median values of parameters with Beta distributions were not yet available. Because of project time constraints, the calculations proceeded with mean values instead of median values for the bulk density (DNSBLK), matrix porosity (POROSITY), residual water saturation (RESISAT), and the van Genuchten alpha (VGALPHA). When all median values were available, the median parameter value simulation was then performed.

In Table 12-4, the actual median value, the value used in the 36 sampling sets, and the relative change between them are as shown for all Beta distribution parameters that were not sampled. Although large relative changes in the residual water saturation are shown in Table 12-4, the absolute change is small, and so we believe the error to be acceptable. Other large relative changes are noted in the POROSITY of the TCW and TSV, and the VGALPHA of the PTn. The influence of these changes is hard to estimate, but given the vertical distance of the TCW and PTn from the repository and the relatively small size of the TSV, the overall impact is presumably small.

Table 12-4. Median Values of Non-Sampled Parameters Using the Beta Distribution

Material ID	Parameter	Value Used	Median	% Change
CHNV	DNSBLK	1.838×10^3	1.816×10^3	-1.2%
CHNZ	DNSBLK	1.746×10^3	1.743×10^3	-0.2%
PTN	DNSBLK	1.714×10^3	1.706×10^3	-0.4%
PPW	DNSBLK	1.993×10^3	1.934×10^3	-3.1%
TCW	DNSBLK	2.366×10^3	2.402×10^3	1.5%
TSV	DNSBLK	2.308×10^3	2.318×10^3	0.4%
TSWC	DNSBLK	2.258×10^3	2.258×10^3	0.0%
CHNV	POROSITY	3.310×10^{-1}	3.357×10^{-1}	1.4%
CHNZ	POROSITY	3.060×10^{-1}	3.060×10^{-1}	0.0%
PTN	POROSITY	4.210×10^{-1}	4.252×10^{-1}	1.0%
PPW	POROSITY	2.920×10^{-1}	2.963×10^{-1}	1.5%
TCW	POROSITY	8.700×10^{-2}	6.875×10^{-2}	-26.5%
TSV	POROSITY	6.500×10^{-2}	5.457×10^{-2}	-19.1%
TSWC	POROSITY	1.390×10^{-1}	1.336×10^{-1}	-4.0%
CHNV	RESISAT	9.700×10^{-2}	3.662×10^{-2}	-164.9%
CHNZ	RESISAT	1.210×10^{-1}	4.168×10^{-2}	-190.3%
PTN	RESISAT	1.540×10^{-1}	9.036×10^{-2}	-70.4%
PPW	RESISAT	6.900×10^{-2}	6.219×10^{-2}	-11.0%
TCW	RESISAT	2.100×10^{-2}	3.716×10^{-3}	-465.2%
TSV	RESISAT	1.180×10^{-1}	4.108×10^{-2}	-187.3%
TSWC	RESISAT	4.500×10^{-2}	2.124×10^{-2}	-111.9%
CHNV	VGALPHA	-1.644	-1.750	6.1%
CHNZ	VGALPHA	-2.270	-2.320	2.1%
PTN	VGALPHA	-1.134	-1.298	12.6%
PPW	VGALPHA	-1.777	-1.781	0.2%
TCW	VGALPHA	-2.094	-2.066	-1.4%
TSV	VGALPHA	-2.624	-2.511	-4.5%
TSWC	VGALPHA	-1.885	-1.953	3.5%

12.1.3 Intermediate Results

The fluid flow and temperature results of all 38 simulations for both the horizontal and vertical emplacements are presented here. In most cases, a general trend in behavior can be seen when all simulations are compared on a single plot. This pattern is essentially the most probable system response, given the underlying modeling assumptions and existing data. In the discussion that follows, general trends and behavior patterns are discussed in detail. Abnormal or unusual behavior is noted and discussed as necessary.

Within the repository, grid block sizes are relatively large, containing a number of waste packages, the void space between the waste packages and the rock, and the rock that separates the rooms. Therefore, variables such as repository pressure, saturation, and temperature should be regarded as average values of the system within the element. Repository variables may fluctuate significantly within an element. Temperature is of particular concern, because the waste packages will generally be much hotter than the average grid block temperature. Temperature is an important parameter to the waste package corrosion submodel, so a method of computing the waste package temperature based on the average grid block temperature was developed. This technique is presented in Section 12.2.

In an attempt to approach steady state conditions before inserting the waste in the model, a 1000-yr equilibrium period was run. The results, as presented, do not include the equilibrium portion of the simulation. Instead, the state of the system at the end of the 1000-yr equilibration period is treated, and referred to, as the initial conditions. Note that the initial conditions at the time of waste disposal may be quite different than the "pre-equilibrium" initial conditions discussed in the previous section.

Cumulative flow and flow rates in the vertical direction are computed by integrating the flow field over one-half the repository footprint. The flow area of the horizontal emplacement repository is 456.36 m by 263.47 m, or 120,237 m². The vertical emplacement repository is 456.36 m by 298.65 m, or 136,292 m². In the horizontal direction, the flow field is integrated over a plane that runs along the edge of the repository, and at a distance 2.4 km from the repository boundary.

Repository with Horizontal Emplacement. The repository temperature, water saturation, fluid pressures, and gas composition of the repository with horizontal emplacement are presented in Figures 12-10 and 12-11. These variables are shown at both the center and edge of the repository (grid block locations [1,19] and [29,19], respectively, in Figure 12-4). Fluid flow through the repository is presented in Figure 12-12. All results are presented in a semi-log format to analyze the repository's response to heat generated by the waste at early times.

Repository Temperature. Heat production is greatest after initial waste disposal. As the waste decays, the energy output declines, as shown in Chapter 4, Figure 4-13. The response to this type of thermal loading is shown in Figures 12-10a and 12-10b. The repository temperature increases from an initial value of 26°C to a maximum value of 90°C to 94°C, and then falls slowly. The peak temperature is reached at the center of the repository, roughly 30 yr after the waste disposal. The temperature in the center of the repository remains above 80°C for around 600 yr, then begins to drop at more rapid pace. Maximum temperatures are about 25°C lower at the edge of the repository, but the overall behavior is nearly the same.

Heat produced by the waste is transported away from the repository convectively through fluid migration, and conductively through the rock matrix. Flow properties of the geologic barrier, which are sampled, result in very different flow fields, and thus different amounts of convectively transported heat. The thermal conductivity and specific heat of the rock are not sampled though, so each simulation has approximately the same amount of energy transported conductively. Because the temperature profiles show very little variation between sample sets, it is apparent that the dominant mechanism for energy transport is conductive flow through the rock matrix.

Repository Water Saturation. Initial matrix water saturation varies from 0.65 to 1.00 at both the center and edge of the repository, Figures 12-10c and 12-10d. Within 10 yr, the elevated temperatures and continued energy output begin vaporizing the water contained in the matrix pores. In most simulations, water vaporizes more quickly than it is replenished, leading to a drop in matrix water saturation. The drop is larger and sustained for a longer period of time at the center of the repository because of higher temperatures there. At the repository edge, the matrix water saturation quickly recovers from the initial drop, and then, in most cases increases to levels that far exceed the initial sat-

12. Complex Consequence Modeling

Figure 12-10. Repository temperature, matrix water saturation, and fracture water saturation at the repository center and edge for horizontal emplacement.

(a) Center

(b) Edge

(c) Center

(d) Edge

(e) Center

(f) Edge

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Figure 12-11. Repository water pressure, gas pressure, and air mass fraction at the repository center and edge for horizontal emplacement.

uration. This is classical heat pipe behavior (Wilson et al., 1994, Chapter 10.1), where water vaporizes near the energy source, is transported in the gas phase, and then condenses in cooler regions of the repository and surrounding rock.

The initial water saturation of the repository fractures is below the residual water saturation, 0.04, in all but one of the simulations (Figures 12-10e and 12-10f). When the water saturation is less than the residual saturation, water in the fracture is hydraulically immobile. Fracture pore spaces begin to saturate only after enough water is present to completely saturate the rock matrix (discussed in Section 12.1.1). After about 3000 yr, a number of runs show a rapid increase in both matrix and fracture water saturation. The surge in saturation is a response to water infiltrating from the surface. The increased flow is more prevalent in the center of the repository because of the enhanced surface infiltration cell, located directly above the repository.

Repository Pressure. Following the 1000-yr equilibration period (time = 0), the repository water pressure in most simulations is slightly negative, somewhere between 0 and -4 MPa (Figures 12-11a and 12-11b). Water saturation changes resulting from vaporization are accompanied by a drop in water pressure due to capillary effects. The water pressure curves are very similar in behavior to the water saturation curves due to relatively small fluctuations in gas pressure (Figures 12-11c and 12-11d).

Repository Gas Composition. The gas phase is assumed be a mixture of air and water vapor in a state of thermodynamic equilibrium with the liquid phase. The initial composition in terms of mass fraction is roughly 92% air and 8% water vapor, as shown in Figures 12-11e and 12-11f. As the temperature rises and liquid water is vaporized into the gas phase, air is displaced from the repository and reduces the air content in the gas phase. The air mass fraction reaches a minimum value of 30% as the temperature peaks in the center of the repository. As the repository cools, air returns by diffusion and advection, eventually reaching the initial state. At the edge of the repository, water vaporization is substantially lower. The air content of the gas phase is consequently much greater near the edge of the repository than at the center.

Oxygen is a key element affecting the corrosion resistance of the waste container. Generally, anoxic corrosion rates are substantially less than oxic rates. Assuming the mole fraction of oxygen in air is 21%, the minimum oxygen content in the repository is 7% by mass and 4.4% by moles. Such low oxygen levels will likely inhibit the corrosion process and lengthen the life of the waste package (Section 11.1). In addition, these results show changes only in gas composition due to phase changes and do not include oxygen consumption caused by corrosion of the waste container, biodegradation, or chemical reactions with the waste.

Repository Fluid Flow. Vertical liquid and gas flow at the center of the repository is presented in Figure 12-12. Flow through the top of the repository is shown in Figure 12-12a, and flow through the bottom of the repository is shown in Figure 12-12b. In most simulations, the vaporization process produced a drop in liquid pressure and simultaneous increase in gas pressure. The drop in liquid pressure induced the flow of liquid water towards the repository, while the increase in gas pressure forced gas to flow away from the repository. Because gas moves predominately through the highly conductive fracture network, small changes in gas pressure produce relatively high flow rates in the gas phase. Gas moves both up and down with little indication of gravitational effects. As the repository cools, gas migrates upwards through both the top and bottom of the repository.

In three simulations, liquid flows through the repository in a downward direction as water is vaporized in the repository. Water, which enters the repository from above, flows at a rate exceeding the rate at which it was vaporized. Consequently, the saturation and pressure were not affected by the temperature rise, and the elevated temperatures only enhanced the flow by reducing the viscosity and expanding the water.

Water Infiltration. The infiltration rate and cumulative volume of water that is infiltrated is shown in Figure 12-13. Water injected at the surface is shown in Figure 12-13a, water passing through the TCw into the PTn is shown in Figure 12-13b, and water flowing out of the PTn into the top of the TSw is shown in Figure 12-13c. In several simulations, the surface infiltration rate exceeded the hydraulic conductivity of the TCw, causing the rock matrix to saturate (Figure 12-14). Once the matrix is water saturated, water flows through the fracture network producing a sharp increase in the infiltration rate in both the TCw and PTn. Cumulative flow through the TCw was only slightly less than the cumulative volume injected, indicating the storage capabilities of the TCw are small in comparison to the

(a) Repository Top

(b) Repository Bottom

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Figure 12-12. Vertical liquid and gas flow at the center of the repository, top and bottom.

12. Complex Consequence Modeling

(a) Surface

(b) TCw

(c) PTn

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Figure 12-13. Infiltration rate and cumulative volume of water that is infiltrated for the surface, TCw, and PTn.

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Figure 12-14. Average water saturation for TCw and PTn.

cumulative volume injected. In contrast, the PTn matrix porosity is much larger than that of the TCw, so water saturation changes in the PTn substantially reduced the volume of water entering the TSw.

Deep Percolation. Water flowing from the surface to the depths of the repository and beyond is referred to as deep percolation and is shown in Figure 12-15. In most simulations, deep percolation consisted of water slowly moving downward through the rock matrix. There were however, several runs in which water began to flow through the fracture network, leading to much larger volumes of water passing through the repository. Fracture flow was focused in the center of the repository directly beneath the enhanced infiltration cell.

The repository's influence on percolating water is imperceptible after the first 1000 yr. Water flow rates and cumulative water flow are virtually identical through the top and bottom of the repository (Figures 12-15a and 12-15b). As in the TCw, this condition shows that water storage in the repository is small relative to the volume of water percolating through it. In contrast to the TCw, the repository has a large pore volume capable of storing large amounts of water. The total porosity of the repository is much larger due to the excavation of disposal rooms and passageways. The repository does not retain water in this void space because it behaves and was modeled as a system of large fractures. Water flows easily through this void space and is not held by capillary forces.

Very little of the water injected at the surface actually descends to the water table in the 10,000-yr simulation period (Figure 12-15c). In fact, the cumulative flow of water at the water table was positive, or upward in most simulations. The upward movement of water is a response to vaporization in the repository and the subsequent draw of water towards it. In a couple of simulations water flow did increase at the water table near the end of the simulation. Other runs also appear to be on the verge of a large increase. Had the computations been run another 10,000 yr or more, the water flow rates at the water table would most likely have increased dramatically in many of the simulations.

Liquid Water Flow. The cumulative liquid flow of water at the end of the 10,000-yr period is given in Table 12-5. These results include only the 36 sample sets. The mean and median values represent the mean and median of the 36 sample sets, not the mean and median input parameter results.

In the vertical direction, water flow decreases with depth (Table 12-5). At the water table, the median value is positive demonstrating that the cumulative flow of water at the water table was typically upward. Horizontally, water flow at the edge of the repository was substantially less than vertical flow (Table 12-5b). At the 2.4-km boundary, the horizontal flow of water was even less; in most runs, horizontal water flow at the 2.4-km boundary was nearly zero. Horizontal flow would have been more influential had the formation dip been included in the analysis.

12. Complex Consequence Modeling

(a) Repository Top

(b) Repository Bottom

(c) Water Table

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Figure 12-15. Water flow rate at the (a) top of repository, (b) bottom of repository, and (c) water table.

Table 12-5. Cumulative Water Flow (m³) for the Horizontal Emplacement Repository Design

	Minimum	Maximum	Mean	Median	Standard Deviation
Vertical Water Flow in the Repository Footprint					
TCw	-3.16×10^6	-6.88×10^3	-9.98×10^5	-8.10×10^5	7.08×10^5
PCn	-2.84×10^6	-2.28×10^4	-5.67×10^5	-4.84×10^5	5.74×10^5
Top of Repository	-2.26×10^6	-1.14×10^4	-3.55×10^5	-2.28×10^5	4.46×10^5
Bottom of Repository	-2.21×10^6	1.38×10^4	-3.08×10^5	-1.70×10^5	4.42×10^5
Water Table	-1.08×10^6	1.63×10^5	-1.00×10^5	1.93×10^4	3.08×10^5
Horizontal Water Flow at the Repository Edge					
TCw	-1.14×10^5	-1.64×10^3	-2.18×10^4	-1.26×10^4	2.40×10^4
PTn	-1.31×10^5	-1.93	-8.73×10^3	-1.04×10^3	2.23×10^4
TSw	-2.46×10^5	8.17×10^3	-1.23×10^4	-3.50×10^2	4.21×10^4
TSv	-1.22×10^3	3.26×10^2	-2.68×10^1	3.76×10^1	2.79×10^2
CHnv	-2.05×10^3	1.38×10^5	4.06×10^3	7.90×10^{-1}	2.30×10^4
CHnz	-1.88×10^4	9.08×10^3	-1.82×10^1	2.25×10^2	3.60×10^3
Horizontal Water Flow at the 2.4-km Boundary					
TCw	-4.12	8.00×10^1	4.61	-4.06×10^{-1}	1.53×10^1
PTn	-3.42×10^1	5.30	-9.50×10^{-1}	-2.22×10^{-2}	5.83
TSw	-3.79×10^1	2.79×10^1	-6.67×10^{-1}	6.26×10^{-3}	8.27
TSv	-3.72×10^{-2}	1.41×10^{-1}	2.18×10^{-2}	1.56×10^{-2}	2.80×10^{-2}
CHnv	-1.52×10^3	1.49×10^{-1}	-4.22×10^1	6.02×10^{-4}	2.53×10^2
CHnz	-2.74×10^1	1.88	-5.65×10^{-1}	1.24×10^{-1}	4.64

Gas Flow. Gas flow in and around the repository is one of the most interesting aspects of this study. The flow behavior of the gas phase is shown by plotting the gas-flow field in the fracture continuum of a single run at different times (Figure 12-16). The vector plots are presented on the computational mesh shown in Figure 12-4 and, thus, are not to scale. The elements on the right side of the mesh are much larger than the elements in the repository. Many of these elements are also a good distance from the repository, resulting in small gas velocity vectors. Most of these velocity vectors are too small to show up on the plot, but they are non-zero.

At the start of the simulation (Figure 12-16a), very little gas is flowing anywhere in the problem domain. In 10 yr (Figure 12-16b), water vaporization elevates the gas pressure in the repository, forcing gas to flow away from the repository in all directions. After 100 yr (Figure 12-16c), the vaporization process continues but at a much lower rate. Velocity vectors are small near the surface because water vapor produced in the repository condenses as the gas moves into cooler regions of the geologic barrier. Eventually, the rock above the repository warms up by means of conduction by the rock matrix and latent heat released from water condensation. At 450 yr (Figure 12-16d), differences in gas density, resulting from temperature and composition variations in the gas phase, force gas to flow to the surface. Gas also flows horizontally towards the hotter regions through more permeable layers such as the PTn. At 1000 yr, warm air rises and is replaced by cool air from below the repository (Figure 12-16e). The cool and relatively dry air is heated, and the vapor content of the gas increases. A large amount of water is converted from the liquid

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(a) 0 yr

(b) 10 yr

(c) 100 yr

(d) 450 yr

(e) 1000 yr

(f) 10,000 yr

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Figure 12-16. Gas flow field in the repository with horizontal emplacement at (a) 0 yr, (b) 10 yr, (c) 100 yr, (d) 450 yr, (e) 1000 yr, and (f) 10,000 yr.

1 phase to the gas phase in this process and transported to the surface, partially explaining the drop in liquid water flow
 2 with depth. This cycle continues through the end of the simulation, as shown in Figure 12-16f.

3
 4
 5 The vertical flow of gas for all 38 simulations is presented in Figure 12-17. Gas flow peaks about 2000 yr after
 6 disposal, except in the repository where flow rates peak with temperature about 30 yr after disposal. Flow rates also
 7 increase with elevation, due to the large volume of gas that flows horizontally into the region above the repository
 8 through the surrounding rock. The cumulative volume of gas flowing both horizontally and vertically at the end of
 9 10,000 yr is summarized in Table 12-6.

10
 11
 12 **Gas Travel Time.** Gas travel time from the repository to the surface was investigated using the particle tracking
 13 program, TRACKER (Rechard et al., 1989). Travel times are presented in the form of a cumulative probability distri-
 14 bution (Figure 12-18), generated from results of the 36 sampling sets. Particles were released in the repository, above
 15 the waste (top) and below the waste (bottom), at both the center and edge of the repository. Release times were at 10,
 16 100, and 1000 yr.

17
 18
 19 Generally, travel times are shortest for particles released after 1000 yr. Figure 12-18 indicates the shortest travel
 20 times probably occur around 2000 yr after disposal. At earlier times, the full effect of thermally induced gas flow has
 21 yet to be realized, so the travel time to the surface is usually longer. However, the fastest particles, those having
 22 travel times less than 10 yr, were released above the waste (top) 10 yr after disposal and pushed to the surface by
 23 water vaporization. Particles released at the same time in the bottom center of the repository were pushed downward,
 24 away from the surface, resulting in much longer travel times than particles released above the waste.

25
 26
 27 **Vertical Emplacement Repository.** From a thermal-hydraulic perspective, the main difference between the
 28 vertical and horizontal waste emplacement repositories is the thermal loading. The thermal loading is slightly less in
 29 the vertical emplacement design because the waste is disposed of in a larger repository. As a consequence, the maxi-
 30 mum temperatures, and most of the thermally driven behavior, were reduced in the vertical emplacement repository.
 31 Another factor contributing to differences between the two repositories is the initial matrix water saturation of the
 32 TSw (prior to the 1000-yr equilibration period). This value was changed by mistake after the horizontal emplacement
 33 simulations, but before the vertical emplacement simulations were run. The correct initial TSw matrix water satura-
 34 tion of 0.65 was used in the horizontal emplacement simulations; an incorrect value of 0.85 was used in the vertical
 35 emplacement design.

36
 37
 38
 39 **Repository Variables.** The repository temperature, water saturation, fluid pressures, and gas composition of the
 40 vertical emplacement repository are presented in Figures 12-19, and 12-20. These parameters are shown in the waste
 41 at both the center and the edge of the repository (grid block locations [1,18] and [19,18] in Figure 12-5). The maxi-
 42 mum temperature at the center of the repository is 82°C to 85°C, and peaks around 30 yr after disposal. At lower
 43 temperatures, less water is vaporized, so the drop in matrix water saturation was not as large as the drop observed in
 44 the horizontal emplacement repository. Other differences attributable to the reduced thermal loading are higher
 45 repository water pressures, lower repository gas pressures, and a higher concentration of air in the gas phase.

46
 47
 48
 49 **Repository Fluid Flow.** The impact of increasing the initial water saturation and decreasing the thermal loading
 50 is shown by comparing the flow of liquid water and gas through the two repositories. In the vertical emplacement
 51 repository (Figure 12-21), the downward flow of water is significantly higher than the horizontal emplacement repos-
 52 itory (Figure 12-12), due to the difference in the initial TSw matrix water saturation. The reduced thermal loading
 53 vaporized less water, resulting in lower repository gas pressures and, therefore, lower gas flow. At later times, gas
 54 flow is driven by temperature gradients instead of water vaporization, so gas flow rates are approximately the same in
 55 both repositories.

56
 57
 58
 59 The cumulative flow of water through the vertical emplacement repository at the end of the 10,000-yr simulation
 60 is summarized in Table 12-7. Like the horizontal emplacement repository, water flow decreases with depth. At the
 61 water table, cumulative downward water flow is approximately one-ninth of the volume injected at the surface. Flow
 62 at the water table was much greater in the vertical emplacement repository because of the additional water in the
 63 TSw.

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Figure 12-17. Flow of gas at (a) surface, (b) TCw, (c) PTn, (d) repository top and, (e) repository bottom for the horizontal repository.

Table 12-6. Cumulative Gas Flow (m³) for the Horizontal Emplacement Repository Design

	Minimum	Maximum	Mean	Median	Standard Deviation
Vertical Gas Flow in the Repository Footprint					
TCw	4.45×10^7	1.31×10^9	3.96×10^8	3.30×10^8	3.10×10^8
PCn	4.42×10^7	1.05×10^9	3.31×10^8	2.68×10^8	2.55×10^8
Top of Repository	3.48×10^7	6.01×10^8	1.89×10^8	1.63×10^8	1.34×10^8
Bottom of Repository	-2.32×10^7	4.92×10^8	1.33×10^8	9.77×10^7	1.23×10^8
Water Table	-2.73×10^4	1.55×10^7	2.88×10^6	1.07×10^6	3.95×10^6
Horizontal Gas Flow at the Repository Edge					
TCw	-1.21×10^9	-7.58×10^7	-3.19×10^8	-2.20×10^8	2.74×10^8
PTn	-4.19×10^8	-9.07×10^5	-6.90×10^7	-1.94×10^7	1.04×10^8
TSw	-1.78×10^{10}	-4.74×10^5	-1.56×10^9	-6.80×10^7	4.05×10^9
TSv	-1.75×10^7	-6.15×10^5	-4.90×10^6	-3.48×10^6	3.88×10^6
CHnv	-1.26×10^7	-1.14×10^4	-2.41×10^6	-9.38×10^5	3.20×10^6
CHnz	-1.89×10^8	-1.99×10^5	-3.64×10^7	-1.42×10^7	4.83×10^7
Horizontal Water Flow at the 2.4 km Boundary					
TCw	-1.80×10^6	-5.76×10^4	-3.35×10^5	-2.45×10^5	3.16×10^5
PTn	-6.18×10^6	-1.58×10^4	-5.93×10^5	-1.05×10^5	1.33×10^6
TSw	-1.60×10^9	-1.10×10^4	-7.25×10^7	-4.18×10^6	2.68×10^8
TSv	-4.14×10^6	-1.04×10^5	-7.58×10^5	-3.82×10^5	9.74×10^5
CHnv	-5.14×10^6	-6.51×10^3	-4.46×10^5	-4.88×10^4	1.11×10^6
CHnz	-8.38×10^7	-1.07×10^5	-7.33×10^6	-8.18×10^5	1.80×10^7

Cumulative gas flow is summarized in Table 12-8. Notice the cumulative flow values in the vertical emplacement repository are very close to the cumulative flow values of the horizontal emplacement repository (Table 12-6). The similarity of results suggest the thermal loading has little effect on gas phase transport over a 10,000-yr time span.

Gas Travel Time. Gas travel time from the vertical emplacement repository to the surface of all 36 sample sets is presented as cumulative probability distribution in Figure 12-22. In general, gas travel times in the vertical emplacement repository are very close to the travel times of the horizontal emplacement repository, indicating again that thermal loading variation has very little influence on gas transport. The increased loading of the horizontal emplacement repository reduced gas travel times but only at early times. For particles released at 100 yr in the center-bottom (c) of the repository, the travel time is much longer in the vertical emplacement repository than in the horizontal emplacement repository. Therefore, the repository's thermal loading can influence gas travel time at early times.

12. Complex Consequence Modeling

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Figure 12-18. Gas travel time from the repository to the surface in the horizontal emplacement repository.

Figure 12-19. Repository temperature, matrix water saturation, and fracture water saturation at the repository center and edge for vertical emplacement.

12. Complex Consequence Modeling

(a) Center

(b) Edge

(c) Center

(d) Edge

(e) Center

(f) Edge

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Figure 12-20. Repository water pressure, gas pressure, and air mass fraction at the repository center and edge for vertical emplacement.

(a) Repository Top

(b) Repository Bottom

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Figure 12-21. Water and gas flow at the center of vertical emplacement repository.

Table 12-7. Cumulative Water Flow (m³) for the Vertical Emplacement Repository Design

	Minimum	Maximum	Mean	Median	Standard Deviation
Vertical Water Flow in the Repository Footprint					
TCw	-3.59×10^6	-4.54×10^3	-1.13×10^6	-9.17×10^5	8.03×10^5
PCn	-3.31×10^6	-3.34×10^4	-6.92×10^5	-5.70×10^5	6.55×10^5
Top of Repository	-3.02×10^6	-6.18×10^3	-6.25×10^5	-5.61×10^5	5.85×10^5
Bottom of Repository	-2.97×10^6	8.70×10^3	-5.95×10^5	-5.24×10^5	5.79×10^5
Water Table	-2.09×10^6	9.09×10^4	-3.51×10^5	-1.10×10^5	5.65×10^5
Horizontal Water Flow at the Repository Edge					
TCw	-1.27×10^5	-1.71×10^3	-2.50×10^4	-1.35×10^4	2.78×10^4
PTn	-1.66×10^5	-1.08×10^1	-1.03×10^4	-1.24×10^3	2.79×10^4
TSw	-7.92×10^5	1.10×10^4	-3.07×10^4	-1.51×10^3	1.32×10^5
TSv	-2.11×10^3	7.29×10^2	-2.30×10^2	6.81	5.58×10^2
CHnv	-4.57×10^3	9.63×10^4	3.20×10^3	3.31×10^{-1}	1.63×10^4
CHnz	-2.78×10^4	5.73×10^3	-1.57×10^3	7.70×10^1	5.41×10^3
Horizontal Water Flow at the 2.4 km Boundary					
TCw	-1.05×10^5	-1.87×10^{-1}	-4.58×10^3	-6.91×10^1	1.77×10^4
PTn	-3.06×10^4	-9.33×10^{-3}	-9.43×10^2	-1.24×10^1	5.09×10^3
TSw	-5.54×10^4	-1.58×10^2	-2.96×10^3	-7.40×10^1	9.48×10^3
TSv	-2.02×10^4	2.28×10^{-2}	-1.18×10^3	-5.31×10^1	3.60×10^3
CHnv	-5.50×10^6	8.55×10^{-2}	-1.82×10^5	-3.88	9.18×10^5
CHnz	-2.37×10^5	3.63×10^{-1}	-1.05×10^4	-1.53×10^1	4.06×10^4

Table 12-8. Cumulative Gas Flow (m³) for the Vertical Emplacement Repository Design

	Minimum	Maximum	Mean	Median	Standard Deviation
Vertical Gas Flow in the Repository Footprint					
TCw	4.44×10^7	1.30×10^9	3.93×10^8	3.30×10^8	3.06×10^8
PCn	4.40×10^7	1.05×10^9	3.31×10^8	2.69×10^8	2.56×10^8
Top of Repository	3.07×10^7	6.05×10^8	1.89×10^8	1.54×10^8	1.40×10^8
Bottom of Repository	4.92×10^6	5.04×10^8	1.42×10^8	1.14×10^8	1.19×10^8
Water Table	-3.47×10^4	1.51×10^7	2.79×10^6	1.01×10^6	3.87×10^6
Horizontal Gas Flow at the Repository Edge					
TCw	-1.10×10^9	-6.93×10^7	-2.92×10^8	-2.01×10^8	2.50×10^8
PTn	-3.94×10^8	-8.36×10^5	-6.42×10^7	-1.79×10^7	9.76×10^7
TSw	-1.78×10^{10}	-4.77×10^5	-1.58×10^9	-6.93×10^7	4.09×10^9
TSv	-1.61×10^7	-6.22×10^5	-4.64×10^6	-3.34×10^6	3.65×10^6
CHnv	-1.22×10^7	-1.09×10^4	-2.33×10^6	-8.76×10^5	3.11×10^6
CHnz	-1.84×10^8	-1.89×10^5	-3.53×10^7	-1.32×10^7	4.71×10^7
Horizontal Gas Flow at the 2.4 km Boundary					
TCw	-1.63×10^6	2.68×10^5	-2.59×10^5	-1.76×10^5	3.31×10^5
PTn	-4.38×10^6	-1.04×10^4	-4.53×10^5	-9.87×10^4	9.73×10^5
TSw	-1.06×10^9	-3.57×10^3	-5.16×10^7	-3.07×10^6	1.78×10^8
TSv	-4.21×10^6	-8.41×10^4	-6.69×10^5	-2.93×10^5	9.60×10^5
CHnv	-4.23×10^6	-6.10×10^3	-3.70×10^5	-4.04×10^4	9.17×10^5
CHnz	-6.90×10^7	-1.01×10^5	-6.09×10^6	-6.71×10^5	1.50×10^7

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Figure 12-22. Gas travel time from the repository to the surface in the vertical emplacement repository.

12.2 Thermal Conduction Calculations for Complex PA

The heat generated by the waste within the disposal containers is significant to the repository environment. A repository design consideration is the spacing of waste containers so that local temperatures from the wastes do not exceed the limits of either the waste forms or the backfill or host rock that surrounds the containers. Values for the heat generated by the wastes are also essential to computations of corrosion rates of the containers.

For the Complex PA, thermal conduction calculations generated data regarding heat output from containers in a waste disposal group. The data were used by the source term submodel, USATCONC (Chapter 11), in conjunction with thermal data calculated by BRAGFLO_T. The thermal conduction data described here were used to scale the thermal values generated by BRAGFLO_T as a means of obtaining increased resolution regarding the temperature at canister walls.

12.2.1 Code Descriptions for Thermal Conduction Calculations (J.W. Berglund)

For the Complex PA, the thermal conduction code, CONRAD was used with BRAGFLO_T results to determine time-dependent temperature distributions near a container and within the repository.

CONRAD, a modified version of the heat-conduction code, COND_1D (used in the 1993 PA), was used to determine near-field temperatures. CONRAD treats thermal conduction in an axisymmetric geometry and allows for radiation heat transport across an air gap. These near-field temperatures were corrected by adding the temperature of the overall repository, which was obtained from the BRAGFLO_T computations. (For the Simple PA [Chapter 13], CONRAD results were combined with repository temperatures calculated with SUMQ_3D [Section 13.2].)

CONRAD is an explicit finite-difference code that is designed to study one-dimensional thermal conduction and thermal radiation in spherical or cylindrical coordinates. CONRAD permits different material properties, heat flux boundary conditions that vary with time, internal thermal sources, and radiative heat transport across an air gap. CONRAD is used to determine the temperature field within and adjacent to a single container.

CONRAD is based on the solution to the thermal conduction equation (Scipio, 1967)

$$\nabla \cdot (K \nabla T) + Q = \rho c \frac{\partial T}{\partial t} \quad (12.2-1)$$

where

- Q = heat rate within the medium,
- c = specific heat,
- ρ = mass density,
- t = time,
- K = thermal conductivity,
- ∇T = gradient of the temperature.

Equation 12.2-1 is solved explicitly using finite-difference approximations to the derivatives along a nonuniform, one-dimensional grid. Decaying heat sources are permitted.

Heat was assumed to be transferred across the air gap that forms between the container and the host rock by thermal radiation only. The values are calculated by solving the equation (Jakob and Hawkins, 1957):

$$q_{1-2} = \frac{\sigma A_1}{\frac{1}{\epsilon_1} + \frac{A_1}{A_2} \left(\frac{1}{\epsilon_2} - 1 \right)} (T_1^4 - T_2^4) \quad (12.2-2)$$

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where

- q_{1-2} = rate of heat transfer between surfaces 1 and 2,
 ϵ_1, ϵ_2 = emissivity of surfaces 1 and 2,
 A_1, A_2 = areas of surfaces 1 and 2,
 σ = Stefan-Boltzmann constant,
 T_1, T_2 = absolute temperatures.

12.2.2 CONRAD Calculations for the Complex PA

As mentioned in Section 12.2.1, the repository field temperatures for the Complex PA were generated using BRAGFLO_T. To obtain the local thermal response within and adjacent to each of the 18 containers used in the horizontal and vertical emplacement configurations, the results from CONRAD calculations for each container were added to the field temperatures.

For the vertical emplacement configuration, all containers were assumed to be circular in cross-section; equivalent round cross-sections based on area were used for cross-sections that were not round. An air gap of 0.025 m between the container and tuff was assumed. For the horizontal emplacement configuration, all containers were circular in cross-section and separated from the tuff by a 1.255-m air gap.

The thermal conduction and radiation properties considered are provided in Table 12-9.

Table 12-9. Thermal Conduction and Radiation Properties

Description	Unit
Thermal conductivity of welded tuff	2.1 W/(mK)
Diffusivity of welded tuff	$9.24 \times 10^{-7} \text{ Wm}^2/\text{J}$
Thermal conductivity of container	0.7 W/(mK)
Diffusivity of container	$4.375 \times 10^{-7} \text{ Wm}^2/\text{J}$
Emissivity of container wall	0.8
Emissivity of welded tuff	0.8
Stefan - Boltzmann constant	$5.6717 \times 10^{-8} \text{ W}/(\text{m}^2\text{K}^4)$
Initial temperature	26°C

Local transient temperatures were computed for each container type with CONRAD. The total temperatures within and near each canister type were then obtained by adding the CONRAD results to the temperature changes calculated by BRAGFLO_T.

12.2.3 Computed Thermal Histories

For the Complex PA, overall repository temperatures were calculated using the BRAGFLO_T code. Temperatures at the repository for the vertical and horizontal configurations are shown in Figure 10a, 10b, 19a, and 19b. The effect of water vaporization is shown clearly by the temperature plateaus at 100°C. To obtain local temperatures within each container, the field temperature computed by BRAGFLO_T was added to the results of the CONRAD calculations for each individual container (18 total; 9 for the horizontal and 9 for the vertical) (Figure 12-23). The calculated CONRAD temperature increments are shown for the container center and wall in Figures 12-24 and 12-25 for the horizontal and vertical emplacements, respectively.

(a) Horizontal Emplacement

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(b) Vertical Emplacement

Figure 12-23. Temperatures for waste parcel walls at center of repository for horizontal and vertical emplacements.

Figure 12-24. Temperature increments for individual containers in the horizontal emplacement at container (a) center and (b) wall.

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Figure 12-25. Temperature increments for individual containers in the vertical emplacement at container (a) center and (b) wall.

12.3 Radionuclide Transport Modeling in Unsaturated Zone

For the Complex PA, radionuclide transport in the unsaturated zone was performed with the NUTS (NUclide Transport System) finite-difference program. The flow fields were calculated with the BRAGFLO_T code (discussed in Section 12.1) and then passed to the NUTS model as input. NUTS, which was originally developed for use by the WIPP Project, was selected for the 1994 PA because of its capability for performing transport calculations in the unsaturated zone in multi-porous media (dual-porosity/dual-permeability). In NUTS, the transport calculation is decoupled from fluid flow. The underlying assumption allowing for decoupling of the flow and transport simulation is that solute concentrations are small and do not affect fluid density or thermal properties. The radionuclide source term for NUTS was provided by USATCONC, discussed in Chapter 11. The release rate from the source submodel is implemented as a point source (injection) in the repository computational nodes.

For each fluid flow run, transport runs were performed for both liquid and gas. Therefore, 74 runs were conducted for the water phase and 74 runs for the gas phase.

12.3.1 Mathematical Model Description

NUTS is a multidimensional, multicomponent transport code with single-porosity, dual-porosity, and dual-permeability capabilities. The model is comprehensive and capable of determining the migration rate, distance, concentration, and level of radioactivity of radionuclides transported from the repository and in the surrounding formations.

Transport in the Liquid Phase.

Transport Mass Balance Equation. For the Complex PA calculations, NUTS was run with dual permeability. In standard dual permeability, the partial differential equations that represent the transport in a fractured porous medium consist of fracture and matrix equations coupled by a transfer function between the two media (Kazemi et al., 1976; Hill and Thomas, 1985; Litvak, 1985; Coats, 1989). The multidimensional difference form of the equations governing the transport of radionuclides in the liquid phase in the dual-permeability formulation (Bear et al., 1993; Shinta and Kazemi, 1993) are as follows:

Fracture:

$$\begin{aligned} \Delta_x [\phi_f S_{wf} K_{wf} \Delta_x C_{nwf}] + \Delta_x [T_{wf} C_{nwf} (\Delta_x P_{wf} - \gamma_{wf} \Delta_x D_f)] + C_{nwf}^* Q_{wf} - \tau_{wm/f} C_{nwm/f} - \\ \phi_m S_{wm} K_{wm/f} (C_{nwf} - C_{nwm}) = \frac{V_R}{\Delta t} \Delta_t [\phi_f S_{wf} C_{nwf} + (1 - \phi_t) \rho_s C_{nsf}] + \\ V_R [\phi_f S_{wf} C_{nwf} + (1 - \phi_t) \rho_s C_{nsf}] \lambda_n - V_R \sum_{j=1}^J \{ [\phi_f S_{wf} C_{nwfpj} + (1 - \phi_t) \rho_s C_{nsfpj}] \lambda_{npj} \} \end{aligned} \quad (12.3-1)$$

$$n = 1, 2, \dots, N$$

Matrix:

$$\begin{aligned} \Delta_x [\phi_m S_{wm} K_{wm} \Delta_x C_{nwm}] + \Delta_x [T_{wm} C_{nwm} (\Delta_x P_{wm} - \gamma_{wm} \Delta_x D_m)] + C_{nwm}^* Q_{wm} + \tau_{wm/f} C_{nwm/f} + \\ \phi_m S_{wm} K_{wm/f} (C_{nwf} - C_{nwm}) = \frac{V_R}{\Delta t} \Delta_t [\phi_m S_{wm} C_{nwm} + (1 - \phi_t) \rho_s C_{nsm}] + \\ V_R [\phi_m S_{wm} C_{nwm} + (1 - \phi_t) \rho_s C_{nsm}] \lambda_n - V_R \sum_{j=1}^J \{ [\phi_m S_{wm} C_{nwmpj} + (1 - \phi_t) \rho_s C_{nsmpj}] \lambda_{npj} \} \end{aligned} \quad (12.3-2)$$

$$n = 1, 2, \dots, N$$

where

C_{pw}	solute concentration of component n [kg/m ³],
C_{nw}	injected or produced solute concentration of component n [kg/m ³],
C_{ns}	sorbate concentration of component n [kg/m ³],
D	depth [m],
K	dispersion coefficient [m ² /s],
N	total number of nuclides,
P	pressure [Pa],
Q	injection/production rate [m ³ /s],
S	saturation, fraction,
t	time [s],
T	transmissibility [m ² /Pa-s],
V_R	grid block volume [m ³],
Δ_t	value at time n+1 – value at time n,
Δ_x	finite difference operator in x-direction,
γ	static pressure gradient [Pa/m],
λ	decay constant [s ⁻¹],
ϕ	porosity,
ρ	density [kg/m ³],
τ	liquid matrix fracture transfer function [m ³ /s],

Subscripts:

f	fracture
m	matrix
m/f	matrix/fracture
n	component number
pj	parent number
s	solid phase (rock)
t	total (fracture + matrix)
w	water phase

For compactness purposes in the above formulations, only Δ_x which represents a central finite-difference operator in x-direction, is written. Similar operators can be included for y- and z-direction. The number of continua in the above formulae is limited to two, i.e., matrix and fracture. Therefore, it is possible to perform single-porosity, dual-porosity, and dual-permeability simulations. In the single-porosity, the calculations can be run either in the fracture or in the matrix continuum. Depending on the flow flux field and whether matrix-matrix flow is assumed, NUTS behaves as dual-porosity when the fracture is the main path for the transport (continuous continuum) and the matrix is dispersed in the fracture as a sink/source term, and a dual-permeability model when appreciable transport can be attributed to the matrix flow. In both dual-porosity and dual-permeability models, matrix-fracture transfer is the coupling transport term between the two continua.

Convective Transport. The second and fourth terms in Equations 12.2-1 and 12.2-2 are the contribution from the convective transport. In the NUTS conceptualization, mass transfer across grid block interfaces is governed by a Darcian transient flow of the liquid phase consistent with BRAGFLO_T. However, the transfer at the fracture/matrix interface is dominated by a semi-steady-state Darcian flow represented by $\tau_{wm/f}$. The magnitude of these flow terms and their idealizations are provided by BRAGFLO_T as volumetric rates.

The x-component of fracture and matrix transmissibilities of the liquid phase (water) T_{wfx} and T_{wmx} are defined as follows:

$$T_{wfx} = \frac{\Delta y \Delta z}{\Delta x} (k\phi)_{fx} \left(\frac{k_r}{\mu} \right)_{wf} \quad (12.3-3)$$

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and

$$T_{wmx} = \frac{\Delta y \Delta z}{\Delta x} k_{mx} \left(\frac{k_r}{\mu} \right)_{wm} \quad (12.3-4)$$

The fracture/matrix transfer function τ for the water is given by

$$\tau_w = \sigma V_R k_m \left(\frac{k_r}{\mu} \right)_{wm/f} \left[P_{wf} - P_{wm} - \gamma_{wm/f} (D_f - D_m) \right] \quad (12.3-5)$$

where

D	depth [m],
K	permeability [m ²],
k _r	relative permeability [dimensionless],
P	pressure [Pa],
V _R	grid block volume [m ³],
γ	static pressure gradient [Pa/m],
Δx	grid block dimension in x-direction [m],
Δy	grid block dimension in y-direction [m],
Δz	grid block dimension in z-direction [m],
μ	viscosity [Pa/s],
σ	shape factor [m ⁻²],

Dispersive Transport. When a contaminant is transported in porous media, the front spreads out beyond the abrupt interface expected only from the convective part of the flow. Among the processes that lead to a smear (S-shape) front are the sorption-desorption process and mixing or dispersion. Dispersion phenomena are classified into

1. Mechanical dispersion, which results from the variation of velocity distribution along the tortuous path of the pore spaces. Heterogeneity introduced by local variations of permeability can also contribute to this kind of dispersion.
2. Molecular diffusion caused by differential tracer concentration. The difference in concentration could be a consequence of any chemical process capable of changing the concentration of the transported nuclide, such as deposition, sorption, solution ion exchange, chemical reaction, and radioactive decay.

In practical application of solute transport, it is customary to include hydrodynamic dispersion (both molecular and hydrodynamic dispersion). Fick's second law of dispersion is utilized in NUTS to describe the dispersion contribution to mass transfer in both fracture and matrix (term 1 in Equations 12.3-1 and 12.3-2). Dispersion here is treated as a tensor with the assumption that the dispersivity corresponds to an isotropic porous media. Bear (1988) has shown that this assumption allows representation of the dispersivity tensor, in terms of six components, by the following matrix,

$$K = \begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix} \quad (12.3-6)$$

The above tensor is symmetric and has the property of $K_{xy} = K_{yx}$, $K_{xz} = K_{zx}$, and $K_{yz} = K_{zy}$. If the coordinate system coincides with the principal axes of dispersion (the medium is assumed to be isotropic with regards to dispersivity), off-diagonal values will be zero in the tensor matrix. Therefore, the dispersion coefficients for the x-direction in the fracture and the matrix (Bear et al., 1993) are

$$K_{fx} = \frac{\Delta y \Delta z}{\Delta x} \left\{ \frac{D_m^*}{\tau^* f} + \frac{1}{\phi_f S_{wf} |\vec{v}_{wf}|} \left[\alpha_{Lf} v_{wfx}^2 + \alpha_{Tf} (v_{wfy}^2 + v_{w fz}^2) \right] \right\} \quad (12.3-7)$$

and

$$K_{mx} = \frac{\Delta y \Delta z}{\Delta x} \left\{ \frac{D_m^*}{\tau_m^*} + \frac{1}{\phi_m S_{wm} |\vec{v}_{wm}|} \left[\alpha_{Lm} v_{wmx}^2 + \alpha_{Tm} (v_{wmy}^2 + v_{wmz}^2) \right] \right\}, \quad (12.3-8)$$

where the terms between brackets are the x-component of the dispersivity tensor and,

- D_m^* = molecular diffusion coefficient [m^2/s],
- τ_m^* = tortuosity [dimensionless],
- α_L = longitudinal dispersivity [m],
- α_T = transverse dispersivity [m],

and the velocity vector $\vec{v}$ is given by

$$|\vec{v}| = \sqrt{v_x^2 + v_y^2 + v_z^2}.$$

where v_x , v_y , and v_z are the velocities [m/s] in x, y, and z directions, respectively. Similar formulations can be written for y and z components of the dispersion tensor.

Dispersion in the fracture and matrix is generally small and can be neglected if the convective part of the transport is dominant. However, for transport in the repository, dispersion could be the major transport term, particularly away from the radioactive source. In either case, dispersion can be a significant means of mass transfer between fracture and matrix (term 5 in Equations 12.3-1 and 12.3-2). The dispersion coefficient for fracture/matrix flow (Bear et al., 1993) is given by

$$K_{wm/f} = \sigma V_R \left\{ \frac{D_m^*}{\tau_m^*} + \alpha_m \frac{|v_{wm/f}|}{\phi_m S_{wm/f}} \right\}. \quad (12.3-9)$$

where,

- $v_{wm/f}$ = velocity of liquid transfer (m/s)
- $S_{wm/f}$ = upstream weighted fracture or matrix saturation [dimensionless]

The shape factor σ above is defined in general from as

$$\sigma = \sum \frac{A_m}{V_m d}, \quad (12.3-10)$$

where

- A_m = the surface area of the face subjected to flow [m^2],
- V_m = the volume of the matrix block [m^3],
- d = the distance between the face and the center of the matrix block [m].

For cubical matrix block, the shape factor (Kazemi et al., 1976) is therefore,

$$\sigma = 4 \left(\frac{1}{L_x} + \frac{1}{L_y} + \frac{1}{L_z} \right), \quad (12.3-11)$$

where L_x , L_y , and L_z are the block dimension in x, y, and z coordinates.

Sorption. Many chemicals might undergo sorption to the solid surface of the matrix rock. This surface phenomenon takes place because of the mass transfer between the solute and the solid surface and is controlled by the chemical properties of both the solid and the solute. Sorption as a retarding factor in the transport front propagation is

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expressed in NUTS through the variables C_{sm} and C_{sf} , which represent the sorbed concentration of the radionuclide per unit rock weight. It is customary to relate C_{sm} and C_{sf} to the solute concentration by some sort of empirical relations called isotherms. As the name implies, these isotherms are no more than the sorbate concentration versus the solute concentration at a constant temperature. The linear sorption isotherm is used in the Complex PA in which the sorbate concentration is related to the solute concentration (Freeze and Cherry, 1979) by

$$C_s^{n+1} = k_d C_w^{n+1} \quad (12.3-12)$$

where

- $n+1$ = implicitness of the concentration (current time step),
 k_d = partition equilibrium constant.

Decay. NUTS simulates decay of first-order chains of the form $A \rightarrow B \rightarrow C \dots \rightarrow N$. The properties of the modeled radionuclides are provided in the input from USATCONC and the differential form of the decay is used (as opposed to the Bateman's equations). The second and third terms of the right-hand side of Equations 12.3-1 and 12.3-2 are the disappearance of radionuclide n by decay and appearance of n from decay of the preceding chain member, respectively. Examination of these terms shows that both adsorbed and dissolved radionuclides contribute to the decay terms. Because of the implicit treatment of the parent contribution into the immediate daughter, the partial differential equations are solved sequentially from the top of each chain. (USATCONC provides the sequential input file.)

Solubility Limit and Precipitation. When groundwater comes in contact with released waste, dissolution of radionuclides begins and continues until equilibrium concentrations are attained or all radionuclides are consumed. The capacity of the groundwater to dissolve radionuclides is controlled by temperature, pressure, and chemical composition. Consequently, there is a solubility limit for each element in the waste. NUTS requires the solubility limit of the elements and allocates the solubility limit for the isotopes according to their mole fractions. The amount of radionuclides in excess of their solubility limit precipitates in the grid block. Precipitate in NUTS undergoes decay, and precipitation is treated as a reversible process. Once the solute concentration drops below the solubility limit, groundwater is allowed to redissolve from the precipitate a mass equivalent of the solubility limit (or lower) of that solute, depending on the abundance of the precipitate.

Source/Sink Terms. Source/sink terms are included in the Complex PA as follows:

1. Variable strength radioactive source from USATCONC for each computational grid block containing a waste.
2. Constant pressure (Dirichlet boundary condition) sinks from BRAGFLO_T at the upper boundary of the simulated domain (emission into the atmosphere).

Temperature Dependency. It is optional in NUTS to consider the temperature dependency of certain parameters, such as solubility of radionuclide, molecular diffusion, and the solute-solid partition coefficients (equilibrium constants). Discussion of implementation and derivation of these parameters will follow in Section 12.3.4.

12.3.2 Transport in the Gas Phase

It is essential in gas transport to consider the chemical interaction between the gas and the porous medium (and its content) in which it flows. This interaction or phase equilibrium can be classified as gas-solid phase equilibrium described by sorption-desorption process and gas-liquid phase equilibrium.

The description of multiphase equilibrium in porous media is complex and requires a compositional simulator that strongly couples the transport with flow equations. This kind of treatment arises because some mixtures like CO_2 + H_2O , can be observed under certain conditions of pressure, temperature and composition, as a single phase, liquid or vapor, two-phase (vapor-liquid or liquid-liquid), or three-phase (vapor-liquid-liquid). To describe such a system appropriately and predict the number of phases in equilibrium, transport in the liquid and gas phases should be deter-

mined simultaneously. In this case, the solute will be partitioned according to its equilibrium constant between the phases in equilibrium.

However, this compositionally equilibrated system requires not only a detailed description of the pressure, temperature and initial composition fields in the computational domain, but also is very demanding with regard to computation time and resources. Consequently, because of data limitations, NUTS considers the porous medium and its fluid content as a retardation factor for the constituents transported by the gas phase (Doctor et al., 1992). The following phenomena are included in NUTS:

1. Solid-gas phase equilibrium is considered by the same linear equilibrium sorption isotherm described above.
2. Liquid-gas equilibrium is modeled through gas solubility in the water as a function of temperature. The equation that describes this equilibrium is

$$K_{LG} = \frac{C_L}{C_G} \quad (12.3-13)$$

where C_L and C_G are the concentration of the solute in the liquid and gas phases, respectively. The value of the ratio is represented by a linear function of temperature

$$\frac{C_L}{C_G} = A - B T \quad (12.3-14)$$

where A and B are the intercept and the slope, respectively. This linear representation is valid only for a limited range of temperature and at low pressure where composition dependency is usually weak.

Because the migration rate in the liquid phase is much slower than in the gas phase, and because the gas and the liquid phases transport are decoupled in NUTS, liquid transport of a constituent abundantly transported by the gas phase will not be tracked. With the above mentioned assumptions, the transport in the gas phase of a dual-permeability system can be described by the following equations:

Fracture:

$$\begin{aligned} & \Delta_x [\phi_f S_{Gf} K_{Gf} \Delta_x C_{nGf}] + \Delta_x [T_{Gf} C_{nGf} (\Delta_x P_{Gf} - \gamma_{Gf} \Delta_x D_f)] + C_{nGf}^* Q_{Gf} - \tau_{Gm/f} C_{nGm/f} - \\ & \phi_m S_{Gm} K_{Gm/f} (C_{nGf} - C_{nGm}) = \frac{V_R}{\Delta t} \Delta_t [\phi_f S_{Gf} C_{nGf} + (1 - \phi_t) \rho_s C_{nsf} \\ & + \phi_f (1 - S_{Gf}) K_{LG} C_{nGf}] + V_R [\phi_f S_{Gf} C_{nGf} + (1 - \phi_t) \rho_s C_{nsf} + \phi_f (1 - S_{Gf}) K_{LG} C_{nGf}] \lambda_n \\ & - V_R \sum_{j=1}^J \left\{ \left[\phi_f S_{Gf} C_{nGfjp} + (1 - \phi_t) \rho_s C_{nsfpj} + \phi_f (1 - S_{Gf}) K_{LG} C_{nGfjp} \right] \lambda_{npj} \right\} n = 1, 2, \dots, N \end{aligned} \quad (12.3-15)$$

Matrix:

$$\begin{aligned} & \Delta_x [\phi_m S_{Gm} K_{Gm} \Delta_x C_{nGm}] + \Delta_x [T_{Gm} C_{nGm} (\Delta_x P_{Gm} - \gamma_{Gm} \Delta_x D_m)] + C_{nGm}^* Q_{Gm} - \tau_{Gm/f} C_{nGm/f} + \\ & \phi_m S_{Gm} K_{Gm/f} (C_{nGf} - C_{nGm}) = \frac{V_R}{\Delta t} \Delta_t [\phi_m S_{Gm} C_{nGm} + (1 - \phi_t) \rho_s C_{nsm} \\ & + \phi_m (1 - S_{Gm}) K_{LG} C_{nGm}] + V_R [\phi_m S_{Gm} C_{nGm} + (1 - \phi_t) \rho_s C_{nsm} + \phi_m (1 - S_{Gm}) K_{LG} C_{nGm}] \lambda_n \\ & - V_R \sum_{j=1}^J \left\{ \left[\phi_m S_{Gm} C_{nGmpj} + (1 - \phi_t) \rho_s C_{nsmpj} + \phi_m (1 - S_{Gm}) K_{LG} C_{nGmpj} \right] \lambda_{npj} \right\} n = 1, 2, \dots, N \end{aligned} \quad (12.3-16)$$

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where subscript G refers to the gas phase, and K_{LG} is the gas-liquid equilibrium constant. The rest of the nomenclatures are defined in Equations 12.3-1 and 12.3-2.

12.3.3 Assumptions and Limitations

Assumptions and limitations of NUTS calculations are as follows:

1. Decoupling of flow and transport equations is permitted because of the dilute solute concentration (does not affect fluid density, viscosity, etc.).
2. Local equilibrium exists between interacting phases.
3. The radionuclides transported by this model are thermodynamically stable within their solubility limit. No gas phase or radionuclides-rich liquid phase is allowed. However, precipitation is possible beyond the solubility limit.
4. Radionuclides are in equilibrium with the precipitate. The precipitation is a reversible process controlled by the solubility limit as an upper bound.
5. Sorption obeys only equilibrium isotherms (linear isotherm is used in these calculations).
6. Dispersion is assumed to obey Fick's second law with dispersivities corresponding to an isotropic porous medium so that it can be represented by two constants in the principal directions of flow.
7. Colloidal transport is not considered in this model.
8. Solubility of each isotope is evaluated as:
$$(\text{Solubility})_{\text{isotope}} = (\text{Mole Fraction})_{\text{isotope}} \times (\text{Solubility})_{\text{element}}$$
9. Gas-liquid equilibrium follows the linear relationship represented by Equation 12.3-13.
10. Gas travels much faster than liquid. Thus, the liquid phase acts as a retarding agent to the constituents transported by the gas phase.

12.3.4 Implementation of Mathematical Model (Computational Model)

Numerical Approach. The transport equations (Equations 12.3-1 and 12.3-2) have $N * G$ unknowns for single porosity and $N * 2G$ unknowns for dual-porosity and dual-permeability formulations, where G is the number of grid blocks in the simulated spatial domain. The system of partial differential equations is strongly coupled due to the contribution of the parent decay to the immediate daughter (the last terms in Equations 12.3-1 and 12.3-2). The sequential method is used to solve the system implicitly. In the sequential method, the solution proceeds progressively from the top of each radioactive chain. Therefore, the contribution to any daughter from parent decay will be available. This method was chosen to avoid inverting a big (for large number of radionuclides) and very sparse matrix in which the bands are not well structured.

Standard Gaussian elimination has been used to invert the numerical matrix. Two optimization techniques are applied to reduce the numerical matrix to a more manageable size. In the first technique, an optimum dimension (in standard ordering) is chosen to define the connectivity of the grid blocks. The guideline of this choice is the minimum number of grid blocks. Hence, for a two-dimensional problem in x and y , the numbering will start from $\min(x,y)$ and proceed to the next dimension. The second technique is included by straightening the numerical matrix diagonals and limiting the calculation in the entries between the uppermost and the lowermost diagonals. Therefore,

for a single-phase system in two dimension, a pentagonal matrix of $IBW \cdot G$ is inverted instead of $G \cdot G$ matrix, where IBW is the band width.

Algorithms for Temperature-Dependent Parameters. With the lack of experimental data on most of the parameters discussed in this section, a preliminary derivation and treatment of temperature dependency will be suggested here. The main objective behind this section is to raise the question of whether it is important to include this obvious dependency, and to suggest some simplified thermodynamic relations to implement it. With the availability of experimental data, one can test these formulations and fine tune them if necessary.

Solubility Limit. Experimental results (Nitsche et al., 1992; Wilson, 1993) showed that the extent to which solid radionuclides can dissolve in water varies with temperature and the chemical composition of the water (e.g., pH of the solution). The equation of equilibrium of radionuclide i can be written as

$$f_i^s = f_i^1 = \gamma_i x_i f_i^o \quad (12.3-17)$$

where f_i^s is the fugacity of the pure solid phase, f_i^1 is the fugacity of the solute in the liquid solution, γ_i is the activity coefficient of the liquid phase, and f_i^o is standard state fugacity to which γ_i refers. From Equation 12.3-17, the solubility x_i can be evaluated

$$x_i = \frac{f_i^s}{\gamma_i f_i^o} \quad (12.3-18)$$

Following Prausnitz et al. (1986), one can show that the fugacity ratio in Equation 12.3-18 can be found from the following relationship

$$\ln \frac{f_i^1}{f_i^o} = \frac{\Delta H_f}{R T_i} \left(\frac{T_i}{T} - 1 \right) - \frac{\Delta c_p}{R} \left(\frac{T_i}{T} - 1 \right) + \frac{\Delta c_p}{R} \ln \frac{T_i}{T} \quad (12.3-19)$$

provided that the temperature of the solution is not far from the triple point, where,

ΔH_f	=	enthalpy of diffusion, J mole ⁻¹
R	=	gas constant, J mole ⁻¹ K
Δc_p	=	heat capacity at constant pressure, mole ⁻¹ K ⁻¹
T	=	temperature, K
T_i	=	triple point temperature, K

However, in this approach, the activity coefficient γ_i data are not available. Unless the solution is assumed to be ideal ($\gamma_i = 1$), this lack of activity coefficient experimental data will be a significant limitation.

Another way to implement the temperature effect on radionuclide solubility is possible by writing the equilibrium equation (Equation 12.3-17) as

$$f_i^s = \phi_i x_i P \quad (12.3-20)$$

where ϕ_i is the fugacity coefficient of the solute i and can be obtained from any equation of state (EOS) and P is the pressure (Pa). The pure solid fugacity f_i^s can be derived from the basic definition of the fugacity to be

$$f_i^s = P_i^s \phi_i^s \exp \left(\int_{P_i^s}^P \frac{v_i^s \partial P}{R T} \right) \quad (12.3-21)$$

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where,

P_i^s	saturation (vapor) pressure, Pa
ϕ_i^s	fugacity coefficient at saturation pressure [dimensionless]
v_i^s	radionuclide molar volume [$\text{m}^3 \text{mole}^{-1}$]

For the solid radionuclides which is incompressible, f_i^s is fairly approximated by P_i^s . However, the fugacity coefficient calculation requires sufficient binary solubilities (radionuclide + water) at different temperatures to obtain the binary interaction coefficients used by the EOS.

In general most of the experimental data needed for such a phase equilibrium calculation are not available. Therefore, a statistical correlation in terms of temperature and pH is adopted for the 1994 PA calculations. The polynomial (Andrews et al., 1994) describing this temperature dependency of the solubility is

$$\ln(S) = c_0 + \frac{c_1}{T} + \frac{c_2}{T^2} + c_3 T + c_4 \ln(T) + c_5 pH \quad (12.3-22)$$

where,

S	Solubility of the radionuclide, gm/m^3
c_{0-5}	Polynomial parameters (constants)

Molecular Diffusion. Experimentally, diffusion is proportional to the concentration difference across a well defined boundary, or more conveniently, to the concentration gradient, $\partial C/\partial x$, where C is concentration in kg/m^3 of the solution. The diffusion rate is also proportional to the cross-sectional area A across which diffusion is realized. If the diffusion rate is written as $\partial m/\partial t$, the mass transferred across the boundary per second, one can arrive to Fick's law of diffusion

$$\frac{\partial m}{\partial t} = -D A \frac{\partial C}{\partial x} \quad (12.3-23)$$

where D is the proportionality constant referred to as molecular diffusion. D can be recognized as the amount of the solute that diffuses across a unit cross sectional area in one second under the influence of unit concentration gradient. Let us consider diffusion across a distance ∂x over which the concentration changes from C to $C - \partial C$. The driving force is the difference in molar Gibb's free energy (g) of the solute at the two concentrations which can be written as

$$S_{C-\partial C} - g_C = R T \ln \left(\frac{C - \partial C}{C} \right) \quad (12.3-24)$$

If we rewrite Equation 12.3-24 for one macroscopic particle (Barrow, 1973), then the energy difference per particle (G) is

$$G_{C-\partial C} - G_C = \Delta G = \frac{R T}{N} \ln \left(1 - \frac{\partial C}{C} \right) \quad (12.3-25)$$

For a small value of $\partial C/C$ the following approximation is valid,

$$\ln \left(1 - \frac{\partial C}{C} \right) = -\frac{\partial C}{C} \quad (12.3-26)$$

therefore,

$$\Delta G = -\frac{R T}{N} \frac{\partial C}{C} \quad (12.3-27)$$

where N is the number of particles per mole. Gibb's free energy change corresponds to the work done in the transfer of one particle across the distance ∂x and can be written as: $\partial G = Fd * \partial x$, where Fd is the driving force, therefore

$$Fd = \frac{\partial G}{\partial x} = - \frac{RT}{N} \frac{1}{C} \frac{\partial C}{\partial x} \quad (12.3-28)$$

The force Fd will be balanced by frictional forces Ff when a certain velocity v is reached. If the particle is assumed to have a spherical shape of radius r , then the frictional forces exerted by the fluid of viscosity μ is defined by Stoke's law as

$$Ff = 6 \pi r \mu v = 6 \pi r \mu \frac{\partial x}{\partial t} \quad (12.3-29)$$

The diffusion velocity increases until $Fd = Ff$. By equating Equations 12.3-28 and 12.3-29 one can arrive at

$$C \frac{\partial x}{\partial t} = - \frac{RT}{6 \pi r \mu N} \frac{\partial C}{\partial x} \quad (12.3-30)$$

In the above equation $C \frac{\partial x}{\partial t}$ is equivalent to $\frac{\partial m}{A \partial t}$ in Equation 12.3-23 since both of them refers to the mass transferred across the boundary cross sectional area A in the time ∂t (note that $C \partial x = \frac{\partial m}{A}$). Therefore comparing Equation 12.3-30 with Fick's law (Equation 12.3-23) will lead to

$$D = \frac{RT}{6 \pi r \mu N} \quad (12.3-31)$$

The major assumption in the above equation is that the particles are spherical and they obey Stoke's law. However, regardless of the shape of the particles, the importance of this equation lies in the fact that $D \propto \frac{T}{\mu}$ therefore, if we have an experimentally measured value of D at specified temperature and viscosity, then one can write

$$\frac{D_m^*(T)}{D_m^o} = \frac{RT / (6 \pi r \mu(T) N)}{RT^o / (6 \pi r \mu^o N)} \quad (12.3-32)$$

and therefore,

$$D_m^*(T) = D_m^o \frac{T}{T^o} \frac{\mu^o}{\mu(T)} \quad (12.3-33)$$

where,

- D_m^o = molecular diffusion evaluated at the reference temperature
- $D_m^*(T)$ = molecular diffusion at temperature T
- μ^o = reference viscosity at T^o
- $\mu(T)$ = solvent viscosity at temperature T .
- T^o = reference temperature

The above derivation is conducted for the liquid phase. However, it is possible from the kinetic-molecular theory of gases to prove that the proportionality in Equation 12.3-33 is also valid for the gas phase.

Sorption. The equilibrium between the solute and the solid phase is dependent on temperature, pressure, and composition of both the solute and the mineral of the rock surrounding the path of the fluid flow. At equilibrium, Gibb's free energy of sorption is

$$\Delta g = -RT \ln K_d. \quad (12.3-34)$$

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However, from basic thermodynamics

$$\Delta g = \Delta H - T\Delta S, \quad (12.3-35)$$

where

g	molar Gibbs free energy
H	molar enthalpy
K_d	solid-solute equilibrium constant
R	universal gas constant
S	molar entropy
T	temperature

Equating and rearranging Equations 12.3-34 and 12.3-35 will lead to

$$\ln Kd = \frac{1}{R} \left[\frac{-\Delta H}{T} + \Delta S \right] \quad (12.3-36)$$

The change in the enthalpy, ΔH and the entropy, ΔS of sorption to go from the reference temperature T^o to the operating temperature T is

$$\Delta H = \Delta H^o + \Delta c_p^o (T - T^o) \quad (12.3-37)$$

and

$$\Delta S = \Delta S^o + \Delta c_p^o \ln \frac{T}{T^o} \quad (12.3-38)$$

In Equations 12.3-37 and 12.3-38, the heat capacity at constant pressure Δc_p^o is assumed to be temperature independent. Substituting Equations 12.3-37 and 12.3-38 in Equation 12.3-36, will result in

$$\ln Kd = \frac{1}{R} \left\{ -\frac{\Delta H^o}{T} + \Delta S^o + \Delta c_p^o \left[\ln \frac{T}{T^o} + \frac{T^o}{T} - 1 \right] \right\} \quad (12.3-39)$$

The third term on the right-hand side of Equation 12.3-39 is small and can be neglected to simplify the equation to

$$\ln Kd = \frac{1}{R} \left[-\frac{\Delta H^o}{T} + \Delta S^o \right] \quad (12.3-40)$$

where ΔH^o and ΔS^o are the enthalpy and entropy of sorption at reference temperature, T^o , respectively. If we write Equation 12.3-40 for two temperatures T_1 and T_2 and eliminate $\Delta S^o/R$ from the two equations, we can find

$$\ln \left(\frac{Kd_2}{Kd_1} \right) = \frac{\Delta H^o}{R} \left[\frac{1}{T_1} - \frac{1}{T_2} \right] \quad (12.3-41)$$

Equation 12.3-41 if rearranged will lead to

$$Kd_2 = Kd_1 \exp \left[\frac{\xi(T_2 - T_1)}{T_2 T_1} \right] \quad \text{where } \xi = \frac{\Delta H^o}{R} \quad (12.3-42)$$

In the above formulation, Kd_1 and Kd_2 are partition equilibrium constants at temperatures T_1 and T_2 , respectively, R is the gas constant, and ΔH^o is the enthalpy of sorption at reference temperature T^o .

12.3.5 Applied Model

Spatial Discretization and Model Geometry. The geometry of the transport model is identical to that of BRAGFLO_T. The three-dimensional spatial domain is described by two dimensions with element flaring. Upstream weighted concentration in five-point finite-difference approximation is used to discretize the differential equations. The central finite-difference operator is used in spatial discretization. The resultant system of discretized fracture and matrix equations is fully coupled by the transfer function (τ^*C). A more compact form of this system is

$$A x = B \quad (12.3-43)$$

The coefficient matrix A is a banded pentagonal block matrix. Each submatrix has two entries for each component, one for the fracture and one for the matrix. The main diagonal submatrix, however, has four entries (fracture and matrix contribution in each equation). The right hand side B is the vector submatrix of two entries, fracture and matrix. The solution vector x is therefore,

$$x = A^{-1} B \quad (12.3-44)$$

where the inverse matrix A^{-1} is evaluated by Gaussian elimination.

Temporal Discretization. The backward finite-difference operator is utilized in temporal discretization. In order to develop a fully implicit system of equations, each time-dependent variable is dealt with implicitly. Because of the decoupled structure of this calculation (transport follows the flow), communication between NUTS and BRAGFLO_T is achieved by the overall modeling system, CAMCON. BRAGFLO_T output in the database provides NUTS with the required time-dependent parameters. These parameters are velocity at the grid block interfaces, porosities, water or gas saturations, production/injection rates, temperatures, and viscosities. For consistency purposes, the time step size in NUTS is also set to be identical with that of BRAGFLO_T.

Initial and Boundary Conditions. The objective of most numerical solutions is to determine unknown functions that satisfy a given set of partial differential equations in a given domain and at given points at the boundary of that domain. Equations 12.3-1 and 12.3-2 are second order partial differential equations and, therefore, two boundary and/or initial conditions are required to solve each equation. The initial concentrations in both fracture and matrix are initialized to zero, i.e., $C_n(x,y,0) = 0$. In the source submodel, however, the boundary conditions are treated differently, as mentioned in Chapter 11.

Because the external boundary conditions in the flow model (BRAGFLO_T) are set to be no-flow boundaries, the advective part of the differential equation will consistently be zero. However, the dispersive term of the equation is independent of the advection flux (depends on concentration gradient) and its value needs to be specified at the boundaries. For the two-dimension spatial domain described in Sections 12.3, a non-transporting (zero concentration gradient) boundary is assumed.

Interfacing with the Source Submodel (USATCONC). The source submodel, USATCONC is included in NUTS as an internal point source (mass flux boundary) for all the nodes that represent the hypothetical repository. USATCONC calculates the transport inside the canisters and in the possible backfill surrounding the waste parcel. In the liquid phase transport, the source submodel is called within the main time loop of NUTS. Total time, time step size, grid block temperature, concentration in the fractures, and the total mass flux of the repository grid block are fed into USATCONC in each time step. The total mass flux is used in the source submodel to transport the released radionuclide by advection out of the repository. Because USATCONC is conceptualizing one-dimensional flow, this flux is calculated by NUTS with the assumption that a steady-state flow prevails in the grid block. If this is the case, the total flux passed through each canister is equivalent to the total flux leaving the grid block from both the matrix and fracture. The mass (kg/s) transported by USATCONC out of its boundary is reinjected in NUTS as a source term for the transport in the spatial domain. In the gas phase transport calculation, only ^{14}C is transported. Like the liquid transported radionuclides, ^{14}C flux is calculated in the source submodel and passed to NUTS for calculating gas transport.

Material Properties. For dual-permeability simulation runs in NUTS, three sets of material properties are required: rock matrix properties, fracture properties, and radionuclide properties. Fracture and matrix properties include, porosity, grain density, tortuosity, longitudinal dispersivity, transverse dispersivity, and the shape factor σ . Radionuclide properties include half-life, molecular or atomic weight, element solubility, specific activity, chains description, molecular diffusion, and gas-liquid and liquid-solid equilibrium constants. The shape factor is calculated by BRAGFLO_T from the fracture frequency (sampled parameter) using Equation 12.3-11 and passed along with the porosity (time-dependent property) to NUTS. The remaining properties are read from the CAMCON system data base. The dispersivities used in this year's calculation are sampled parameters that range from 5% to 20% of the hydrological distance between the center of the hypothetical repository and the ground surface. Linear partition coefficients (K_d) are used. The only sampled transport parameters, besides the dispersivity percentage mentioned above, are K_d 's for plutonium and neptunium in devitrified tuff and for uranium and neptunium in zeolitic tuff. The mean value is used for the rest of the unsampled properties.

A total of 11 radionuclides were transported in the liquid phase and one radionuclide is transported in the gas phase. The three isotope chains and the five individual isotopes are as follows:

Radionuclides Transported in Liquid Phase:

Radionuclide Transported in Gas Phase:

12.3.6 Intermediate Results for Unsaturated Zone Transport

Liquid Phase Transport. As expected, no measurable releases were observed leaving the surface of the 2400-m boundary within the unsaturated zone after 10,000 yr. Because of the horizontal layering and symmetrical mesh used for the conceptual model description, as well as the water flow associated with the rainfall percolation, the solute escaping the waste parcels generally flowed down toward the water table. This is especially true after the first 1000 yr, when the repository has cooled enough to minimize temperature-related effects such as liquid phase and density changes. Sections 12.4.2 through 12.4.4 discuss in detail the releases to the water table and how the output from NUTS was coupled to the STAFF3D saturated zone transport model.

Gas Phase Transport. Carbon-14 was the only isotope considered for NUTS gas transport for the 1994 PA. The amount of ${}^{14}\text{C}$ released from the waste packages (source model) was minimal, complying with the limits set by 40 CFR 191 before transport out of the repository region (see Chapter 15, Figure 15.2-7b). Consequently, ${}^{14}\text{C}$ releases at the surface were negligible for the 10,000-yr regulatory period.

12.4 Transport Modeling in Underlying Aquifer

Groundwater flow and radionuclide transport modeling in the saturated zone beneath the repository was performed with the STAFF3D (Solute Transport And Fracture Flow in 3 Dimensions) finite-element program. STAFF3D can calculate either Darcy fluid flow or radionuclide transport in either two or three dimensions with (saturated) or without (unsaturated) water table conditions and with either single porosity or dual porosity (Bear and Braester, 1972) idealization. In this performance assessment, the dual porosity conceptual model was used for both the flow and transport with water table conditions. A variable fluid density capability is also available but was not used.

In the dual-porosity approach, the system is assumed to contain numerous fractures, and the domains of both the fractures and porous rock matrix can be represented as two overlapping continua, each filling the entire space. Advective transport occurs only in the fracture domain. Solute exchange between the fracture and matrix occurs due to diffusion at the fracture matrix interface. For this analysis, the flow and transport could be uncoupled and were run separately based on the assumption that solute concentrations are small and do not affect fluid density or flow properties. The radionuclide source was implemented in this analysis at several interior grid points using time dependent, mass flux boundary conditions or injection wells. For this performance assessment the rate histories were estimated using the NUTS code as described in Section 12.3. The associated fluid flow is assumed to have a negligible effect on the aquifer flow; only the solute mass was injected.

12.4.1 Mathematical Model Description

STAFF3D is a finite-element code designed to simulate groundwater flow and solute transport in fractured or granular aquifers with water table boundary conditions (Huyakorn et al., 1992) in either two or three-dimensions. The original 2D version was developed through a joint effort by HydroGeoLogic, Inc. and the International Ground Water Modeling Center of the Holcomb Research Institute. Improved versions of the code have since become commercially available through HydroGeoLogic: the current 3D version is Version 2.0. Changes to the code were made by Sandia to accommodate CAMCON input/output requirements and to tailor the code inputs to the secondary database for the Waste Isolation Pilot Plant (Rechard et al., 1989); these changes also apply to the 1994 PA.

Mass Balance Equation for Flow.

Fracture domain. The governing equation for saturated-unsaturated flow in the fracture domain can be written per unit total (bulk) volume as

$$\frac{\partial}{\partial x_i} \left[\phi_f K_{ij} k_{rw} \frac{\partial h}{\partial x_j} \right] = \phi_f \eta \frac{\partial h}{\partial t} - q - \Lambda \quad (12.4-1)$$

$$\eta = S_w S_s + S_y \frac{dS_w}{dh} \quad (12.4-2)$$

$$S_s = \rho_w g (\phi \beta_c + \alpha_c) \quad (12.4-3)$$

where,

ϕ_f	fracture porosity, [1]
h	hydraulic head, [m]
K_{ij}	saturated hydraulic conductivity tensor of the fracture, [m/s]
k_{rw}	relative permeability of the water phase [1]
x_i	a set of orthogonal spatial coordinates [m]
q	volumetric flow rate via sources/sinks [$\text{m}^3/(\text{s} \cdot \text{m}^3)$]
Λ	volumetric rate of fluid transfer from porous matrix [$\text{m}^3/(\text{s} \cdot \text{m}^3)$]
S_s	specific storage [1/m]

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1	S_y	specific yield [1]
2	S_w	water phase saturation [m^3/m^3]
3	ϕ	porosity of the fracture [1]
4	ρ_w	density of water [kg/m^3]
5	α_c	coefficient of compressibility of the fracture domain [$\text{kg}/\text{m}\cdot\text{s}^2$] $^{-1}$
6	β_c	coefficient of compressibility of the water [$\text{kg}/\text{m}\cdot\text{s}^2$] $^{-1}$

To solve the variably saturated flow problem, it is also necessary to specify the relationship of relative permeability versus water phase saturation and pressure head versus water phase saturation. Two alternative functional relations can be used. These are given by (Brooks and Corey, 1966):

$$k_{rw} = S_e^n \quad (12.4-4)$$

and (van Genuchten et al., 1977);

$$k_{rw} = S_e^{1/2} \left[1 - (1 - S_e^{1/\gamma})^\gamma \right]^2 \quad (12.4-5)$$

$$S_e = (S_w - S_{wr}) / (1 - S_{wr})$$

where, η and γ are empirical parameters and S_e is the effective water and S_{wr} is the residual; water saturation.

The relationship of pressure head, ψ , versus water saturation is described by the following function (van Genuchten et al., 1977; Mualem, 1976):

$$\frac{S_w - S_{wr}}{1 - S_{wr}} = \begin{cases} \frac{1}{\left[1 + (\alpha|\psi - \psi_a|)^\beta \right]^\gamma} & \text{for } \psi < \psi_a \\ 1 & \text{for } \psi \geq \psi_a \end{cases} \quad (12.4-6)$$

where,

α, β	= empirical parameters,
ψ_a	= air entry pressure head,
γ	= usually $1 - 1/\beta$.

The Brooks Corey and van Genuchten functions for moisture retention and relative permeability characteristics can be measured in the laboratory for a given soil.

After the distributions for head and saturation have been determined, Darcy velocity components within the fracture domain are calculated from:

$$V_i = -K_{ij} k_{rw} \frac{\partial h}{\partial x_j} \quad (12.4-7)$$

Porous Matrix Domain. The Λ term in Equation 12.4-1 represents the interaction between the porous rock matrix and fractures. As the hydraulic head is reduced in the fractures, fluid flows from the matrix into the fractures. The flux is a function of the head in the fractures and the head in the porous rock. The hydraulic head distribution in the matrix blocks can be determined by solving a simple one-dimensional flow problem, assuming the permeability of the matrix blocks is small compared with the fracture permeability. For the slab block idealization (Figure 12-7), the equation is as follows:

$$\frac{\partial}{\partial x} \left(K' \frac{\partial h'}{\partial x} \right) = S'_s \frac{\partial h'}{\partial t} \quad (12.4-8)$$

subject to,

$$\begin{aligned} h' &= h'_0 & \text{at } t = 0 \\ K' \frac{\partial h'}{\partial \chi} &= 0 & \text{at } \chi = 0 \\ h' &= h - \zeta K' \frac{\partial h'}{\partial \chi} & \text{at } \chi = B \end{aligned} \quad (12.4-9)$$

where,

- h' = hydraulic head in the matrix block [m],
- K' = hydraulic conductivity [m/s],
- S'_s = specific storage coefficient [1/m],
- ζ = skin resistance parameter (ratio of skin thickness to skin hydraulic conductivity, set to 0 in this analysis).

The volumetric rate of fluid entering the fracture per unit volume of rock matrix is $V_n \sigma$, where

$$V_n = -K' \left. \frac{\partial h'}{\partial \chi} \right|_B \quad (12.4-10)$$

is the boundary condition of the slab block equation, V_n is the Darcy velocity or specific flux at the interface, and σ is the specific surface for a slab block. The volumetric rate of fluid entering the fracture per unit bulk volume, Λ (the coupling term), is therefore

$$\Lambda = V_n \sigma (1 - \phi_f) = \frac{V_n}{B}. \quad (12.4-11)$$

Mass Balance Equation for Dual Porosity Transport.

Fracture Domain. The unsaturated, solute transport mass balance equation assuming constant fluid density, variable porosity and saturation, linear equilibrium sorption, and a fluid and solute source used to model transport in the fractures per unit fracture volume is as follows (see Figure 12-26).

$$\begin{aligned} &\nabla \cdot (D_{II}) \cdot \nabla c_l - V \cdot \nabla c_l \\ &= S_w R_l \frac{\partial}{\partial t} (c_l) - \lambda_l \phi_f S_w R_l c_l + \lambda_p S_w R_p c_p + \frac{q}{\phi_f} (c_l^* - c_l) + \Gamma_l \end{aligned} \quad (12.4-12)$$

where (SI units are shown),

- c_l concentration of the current radionuclide [kg/m³]
- ϕ_f fracture porosity [m³/m³]
- S_w saturation [m³/m³]
- ρ fluid density [kg/m³]
- D_{II} Dispersion tensor [m²/s]
- V Darcy velocity in fracture [m/s] (defined by 12.4-7)
- R_l retardation coefficient for radionuclide l [m³/kg]
- ρ_b bulk density of solid matrix [kg/m³]
- $\lambda_l = \ln(2)/t_{1/2}$ decay constant [s⁻¹]
- $t_{1/2}$ half-life of the current radionuclide [s]
- λ_p decay constant of the parent radionuclide [s⁻¹]
- c_p concentration of the parent radionuclide [kg/m³]
- R_p retardation coefficient of the parent radionuclide l [m³/kg]

12. Complex Consequence Modeling

Figure 12-26. Conceptual hydrologic model of the aquifer.

1 q mass flow rate of fluid at source/sink [$\text{m}^3/(\text{s}\cdot\text{m}^3)$]
 2 c_l^* concentration of solute in fluid source/sink [kg/m^3].
 3

4 The elements of the dispersion tensor, D_{ij} , are defined as (Scheidegger, 1960),
 5
 6

$$D_{11} = \frac{\alpha_L V_1^2 + \alpha_T V_2^2}{|V|} + D_1^*, \quad [\text{m}^2/\text{s}]$$

$$D_{12} = (\alpha_L - \alpha_T) \frac{V_1 V_2}{|V|}, \quad [\text{m}^2/\text{s}] \quad (12.4-13)$$

$$D_{22} = \frac{\alpha_L V_2^2 + \alpha_T V_1^2}{|V|} + D_2^*, \quad [\text{m}^2/\text{s}]$$

17 where α_L and α_T [m] are the longitudinal and transverse dispersivities, and D_1^* and D_2^* [m^2/s] are the effective coefficients of molecular diffusion, including tortuosity effects ($D_1^0 \tau$) where D_1^0 is the free water molecular diffusion of species 1, and τ [dimensionless] is the tortuosity defined as $[L/L_e]^2$, where L designates straight line length and L_e designates actual path length for fluid.
 26

27 The decay constant is
 28

$$\lambda = \frac{\ln(2)}{t_{1/2}}, \quad [\text{s}^{-1}] \quad (12.4-14)$$

32 where $t^{1/2}$ is the half-life of species 1.
 33

34 **Matrix Domain.** The one-dimensional transport equation for slab geometry and no flow conditions in the porous matrix is as follows:
 35
 36

$$\frac{\partial}{\partial x} \left(D' \frac{\partial c_l'}{\partial x} \right) = \phi' R_l' \frac{\partial}{\partial t} (c_l') + \lambda_l \phi' R_l' c_l' - \lambda_p \phi' R_p' c_p' \quad (12.4-15)$$

43 subject to,
 44

$$c_l'(B, t) = c_l(x, y, z, t)$$

$$\frac{D' \delta c_l'(0, t)}{\delta x} = 0$$

52 where,
 53

54 c_l' = dissolved concentration of radionuclide l in matrix [kg/m^3]
 55 D' = effective molecular diffusion for radionuclide l [m^2/s] = $\tau' D_l^0$
 56 ϕ' = porosity of matrix
 57 R_l' = retardation in matrix
 58 = $1 + \frac{\rho_s (1 - \phi') K_d'}{\phi'}$
 59 ρ_s = density of matrix solid [kg/m^3]
 60 K_d' = partition coefficient for matrix [m^3/kg]
 61 τ' = tortuosity of matrix [1]
 62
 63
 64
 65
 66

The dual porosity transport Equations 12.4-12 and 12.4-15 are coupled by equating the flux from fracture, Γ_l , with diffusive flux at the matrix fracture interface as follows:

$$\Gamma_l = - \left(\frac{D' \partial c_l'(x, y, B, t)}{\partial \chi} \right) (1 - \phi_f) \sigma \quad (12.4-16)$$

$$\Gamma_l = \frac{1}{b + B} \left(D' \frac{\partial c_l'}{\partial \chi} \Big|_{\chi=B} \right) \quad (12.4-17)$$

The second $(1 - \phi_f)$ and third (σ) terms on the right-hand side convert the areal flux at the matrix surface to the fracture/matrix control volume of the system.

Assumptions and Limitations. The assumptions and limitations of the model are as follows

- Flow obeys Darcy's law.
- Permeabilities in the porous matrix block are small compared to permeabilities in the fractures.
- Temperature effects on properties are negligible.
- Transport is governed by Fick's law.
- Solute effects on fluid density are assumed negligible so flow and transport can be coupled.
- The dispersivity is assumed to correspond to an isotropic porous medium so that it can be represented by two constants in the principle direction of flow.
- Sorption obeys a linear equilibrium isotherm.
- There is local chemical equilibrium between the liquid and the solid.
- The fracture aperture is small compared to other dimensions in the fracture plane.

Numerical Approach. The finite-element approximation technique applied to both the flow and the transport equations for the fracture domain uses a combined application of the 3D Galerkin and an adaptive upstream-weighted technique (Huyakorn and Nilkuha, 1979; Huyakorn and Pinder, 1983; Huyakorn and Thomas, 1984; Huyakorn et al., 1986, 1987; Panday et al., 1993) designed to overcome oscillations of the numerical solutions when advective terms are dominant. The standard Galerkin approximation technique is used for the one-dimensional matrix flow and transport.

The overall solution procedure is as follows. Matrix computations are performed for heads (for flow) or concentrations (for transport) in both the fracture and porous matrix domains using initial conditions from the previous time step. Tridiagonal sets of algebraic equations for the porous matrix blocks are generated and decomposed using the Thomas algorithm to obtain the relationship between the fluid or solute flux from the porous matrix and the heads or concentrations in the fractures. Using an implicit treatment of the flux terms contributed by the porous matrix, a set of algebraic equations for the fracture domain is generated and solved for nodal values of head or concentration in the fractures using direct banded or ORTHOMIN and Preconditioned Conjugant Gradient (PCG) solvers (Huyakorn et al., 1991). The nodal values are then used to evaluate the fluxes from the porous matrix blocks. Knowing these fluxes, the nodal heads or concentrations values in the porous matrix can be determined by performing the back substitution step of the Thomas algorithm.

Verification. STAFF3D was verified with analytical solutions for both saturated and unsaturated flow and transport. Several of the analytical problems described in the STAFF3D manual have been run and the reported STAFF3D results were reproduced. Analytical problems verified include:

- Well flow in a confined aquifer with parallel fractures (Neuman and Witherspoon, 1969).
- Radial well flow in a confined aquifer with parallel fractures (Bear, 1979).
- Flow to parallel drains in an unconfined aquifer (Bear, 1979).
- Two-dimensional flow in a rectangular soil slab (comparison with VAM3DCG results).
- Longitudinal transport in fractures and transverse matrix diffusion (Tang et al., 1981).

- One-dimensional transport of a three member radioactive decay chain (Coats and Smith, 1964; Lester et al., 1975).
- Two-dimensional transport in a soil slab (comparison with VAM3DCG results).

12.4.2 Applied Model

Model Geometry and Spatial Discretization. The saturated zone underlying the hypothetical tuff site was discretized into a local three-dimensional grid oriented to the north and east to correlate with the Nevada State Plane coordinates. Areally, the grid covers 8,000 m in the x direction (east), and 13,000 m in the y (north) direction for $1.04 \times 10^8 \text{ m}^2$ (Figure 12-27). This grid was chosen to incorporate pressure head data from 28 wells drilled in the Yucca Mountain region, which were used for model calibration. A "pancake" layering in the z direction was developed to include properties of the hydrologic units described in Figure 5-6. Orthogonal grid-block dimensions varied from $150 \text{ m} \times 120 \text{ m} \times 25 \text{ m}$ at the water table beneath the repository region, to $1150 \text{ m} \times 1500 \text{ m} \times 210 \text{ m}$ at the extreme edges of the domain. Additionally, four vertical "fault" regions were included to act as transmissibility barriers for flow calibration. In all, the grid consists of $27 \times 34 \times 21$ grid lines, or 19,278 nodes and 17,160 elements.

Geologic Layer Description and Material Properties. The objective of the aquifer modeling is to approximate flow and transport behavior in the saturated zone within tuffaceous rock beneath a waste disposal repository. To lend credence to the model, certain geologic properties describing the Yucca Mountain region have been used in the model design. This conceptual model is not meant to be a detailed description of the Yucca Mountain aquifer, rather a rough approximation with enough features to adequately describe local flow and transport, and thus radionuclide releases for this performance assessment. The main geologic features incorporated in the model include tilted stratigraphy, vertical fault regions, and a variable water table (unconfined flow) that incorporates a rainfall infiltration model.

Tilted Stratigraphy. The west-to-east dip in the local stratigraphy was achieved by taking a "best fit" plane of the vertical coordinates (mean sea level) at the top of the TSw unit at wells G-1, WT-2, B-1, and H-5. These wells are located just north, south, east, and west of the repository location. The resulting plane has a 4.6° dip west-to-east, and a slight 0.1° dip north-to-south. The remaining geological units were "hung" with a constant thickness from the TSw unit. The material properties used in the dual porosity flow analysis are summarized in Table 12-10. These are the mean values reported in Chapter 7 of TSPA-1993 (Wilson et al., 1994). The vertical fracture conductivity was reduced by a factor of ten to achieve better calibration with the measured well data. The unit thicknesses are the same as those shown in Figure 5-6, with the TRw layer having a thickness of 210 m. Because this model is to be used in saturated zone transport, only the layers that come in contact with the aquifer are modeled. Thus, units TCw and PTn were excluded. The geologic flow properties for units TSwc, CHnv, and PPw were sampled, or varied, for the Monte Carlo analysis. Fracture porosities and conductivities were derived from the bulk conductivities and fracture spacing in a manner consistent with the unsaturated zone flow model (BRAGFLO_T). The resulting model had an aquifer region ranging from approximately 400 m in depth to the west and 900 m to the east, with about 600 m thickness directly under the repository area (Figure 12-28). Tables E.3.1 and E.3.2 (Volume 3, Appendix E) contain a complete listing of the flow properties used for the 36 runs in this performance assessment.

Vertical Fault Regions and Variable Water Table. Examination of the well data revealed several regions of anomalous water table levels (Table 12-11). In the area around the repository site, the water table stays constant at about 730 m, with a slight decrease from west to east. North of the repository area, however, wells G-2 and WT-6 show a water table level of 1029 m and 1035 m. Wells drilled to the west of the repository area (WT-7, WT-10, and H-6) show a piezometric head of 776 m, and well WT-16 recorded the water table at 738 m. Numerous theories have been presented in the Yucca Mountain literature to explain this water table behavior (a complete list of references are presented in TSPA-1993). For this study, a simplified approach using "fault" regions was used to obtain a reasonable fit of the well data. A partially sealing fault was inserted between areas of significantly differing piezometric heads. The fault locations correspond roughly to surface outcrops of some of the major faults in the Yucca Mountain area, namely, Solitario Canyon to the west, Paint Brush to the east, Bow Ridge between them as north - south trending faults, and Drill Hole Wash fault trending northwest - southeast. The Ghost Dance fault was not included in this conceptual model, because the well data indicates it to be nonsealing. These faults are used as transmissibility barriers to flow only, and as such have no dip or strike offset. The water table was allowed to fluctuate as governed by the per-

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Figure 12-27. X-Y "surface" view of STAFF3D grid used for aqueous flow and transport

Table 12-10. Dual-Porosity Flow Parameters Used for STAFF3D Models

Material Number	Unit Number	Rock Type	Material Name	Vector	BLKKGAS	HYCND SAM	HYCND_X	FRACSPAC	POROSITY	SP_STOR	SP_YIELD	DNSBLK
					Bulk Sat Cond Log(m/s)	Matrix Sat Cond Log(m/s)	Matrix Sat Cond (m/s)	Parall. Plate Frac. sp. (m)	Matrix Porosity	Matrix Spec. Storage (1/m)	Matrix Spec. Yield	Bulk Density kg/m ³
9	3	D	TSWC	Mean	-4.62	-9.87	1.353E-10	7.400E-01	0.139	5.544E-06	0.133	2,258
9	3	D	TSWC	Median	-4.77	-10.76	1.738E-11	6.573E-02	0.134	5.518E-06	0.133	2,258
8	4	V	TSW3	Mean	-4.60	-10.58	2.618E-11	8.880E-01	0.065	5.987E-07	0.057	2,308
8	4	V	TSW3	Median	-4.77	-11.02	9.572E-12	7.888E-02	0.055	5.497E-07	0.057	2,318
7	5	V	CHNV	Mean	-4.70	-8.02	9.654E-09	1.618E+00	0.331	8.402E-06	0.299	1,838
7	5	V	CHNV	Median	-5.29	-9.00	9.938E-10	1.418E-01	0.336	8.424E-06	0.299	1,816
6	6	Z	CHNZ	Mean	-5.60	-9.92	1.193E-10	2.059E+00	0.306	1.122E-05	0.269	1,746
6	6	Z	CHNZ	Median	-5.89	-10.75	1.762E-11	1.804E-01	0.306	1.122E-05	0.269	1,743
5	7	D	PPW	Mean	-4.50	-8.54	2.903E-09	3.111E+00	0.292	1.115E-05	0.272	1,993
5	7	D	PPW	Median	-5.80	-8.86	1.379E-09	8.109E-03	0.296	1.117E-05	0.272	1,934
4	9	Z	CFUN	Mean	-6.74	-8.36	4.334E-09	3.111E+00	0.261	8.073E-06	0.246	2,021
4	9	Z	CFUN	Median	-7.01	-8.56	2.750E-09	8.109E-03	0.257	8.055E-06	0.246	2,037
3	8	D	BFW	Mean	-5.21	-9.27	5.390E-10	7.400E-01	0.165	5.666E-06	0.158	2,260
3	8	D	BFW	Median	-5.43	-9.19	6.455E-10	6.573E-02	0.181	5.743E-06	0.158	2,282
2	9	Z	CFMN	Mean	-6.74	-8.36	4.334E-09	3.111E+00	0.261	8.073E-06	0.246	2,021
2	9	Z	CFMN	Median	-7.01	-8.56	2.750E-09	8.109E-03	0.257	8.055E-06	0.246	2,037
1	10	D	TRW	Mean	-5.42	-8.71	1.964E-09	7.400E-01	0.191	5.788E-06	0.182	2,185
1	10	D	TRW	Median	-5.78	-8.97	1.079E-09	6.573E-02	0.200	5.828E-06	0.182	2,193
10-13	0	D	FAULTS	Mean	-12.42	-13.70	2.000E-14	1.000E-01	0.087	7.020E-07	0.085	2,366
10-13	0	D	FAULTS	Median	-12.42	-13.70	2.000E-14	1.000E-01	0.087	7.020E-07	0.085	2,366

Table 12-10. Dual-Porosity Flow Parameters Used for STAFF3D Models (Continued)

Material Number	Unit Number	Rock Type	Material Name	Vector	FHYCND_X Hor. Fracture Hyd. Cond. (m/s)	FHYCND_Z Vertical Fracture Hyd. Cond. (m/s)	FPOROS Fracture Porosity	FSP_STOR Fracture Spec. Storage (1/m)	FSP_YLD Fracture Spec. Yield	FNN Brooks- Corey Exponent	VGALPHA Van Genuch Alpha (1/m)	VGBETA Van Genuch Beta (1/m)	GAMMA Van Genuch Gamma (1/m)	RESISAT Residual Water Sat	PSIA Air Entry Pressure (m)
9	3	D	TSWC	Mean	6.359E-02	6.359E-03	3.77E-04	1.77E-09	1.00	1.00	2.682E-02	1.784E+00	4.394E-01	0.045	0.00
9	3	D	TSWC	Median	1.011E-02	1.011E-03	1.69E-03	7.96E-09	1.00	1.00	1.114E-02	1.617E+00	3.815E-01	0.021	0.00
8	4	V	TSW3	Mean	7.444E-02	7.444E-03	3.40E-04	1.60E-09	1.00	1.00	3.503E-03	2.459E+00	5.934E-01	0.118	0.00
8	4	V	TSW3	Median	1.129E-02	1.129E-03	1.49E-03	7.00E-09	1.00	1.00	3.081E-03	2.002E+00	5.005E-01	0.041	0.00
7	5	V	CHNV	Mean	9.409E-02	9.409E-03	2.10E-04	9.86E-10	1.00	1.00	4.627E-02	2.752E+00	6.366E-01	0.097	0.00
7	5	V	CHNV	Median	7.602E-03	7.602E-04	6.81E-04	3.20E-09	1.00	1.00	1.778E-02	2.077E+00	5.186E-01	0.037	0.00
6	6	Z	CHNZ	Mean	2.790E-02	2.790E-03	8.98E-05	4.22E-10	1.00	1.00	1.489E-02	1.743E+00	4.262E-01	0.121	0.00
6	6	Z	CHNZ	Median	3.531E-03	3.531E-04	3.65E-04	1.71E-09	1.00	1.00	4.789E-03	1.562E+00	3.599E-01	0.042	0.00
5	7	D	PPW	Mean	1.981E-01	1.981E-02	1.58E-04	7.44E-10	1.00	1.00	1.816E-02	7.154E+00	8.602E-01	0.069	0.00
5	7	D	PPW	Median	5.127E-04	5.127E-05	3.09E-03	1.45E-08	1.00	1.00	1.656E-02	5.719E+00	8.251E-01	0.062	0.00
4	9	Z	CFUN	Mean	6.274E-03	6.274E-04	2.85E-05	1.34E-10	1.00	1.00	2.133E-02	3.213E+00	6.888E-01	0.057	0.00
4	9	Z	CFUN	Median	7.733E-05	7.733E-06	1.22E-03	5.72E-09	1.00	1.00	1.689E-02	2.807E+00	6.437E-01	0.056	0.00
3	8	D	BFW	Mean	2.586E-02	2.586E-03	2.41E-04	1.13E-09	1.00	1.00	2.682E-02	1.785E+00	4.399E-01	0.045	0.00
3	8	D	BFW	Median	3.623E-03	3.623E-04	1.01E-03	4.76E-09	1.00	1.00	1.114E-02	1.618E+00	3.819E-01	0.021	0.00
2	9	Z	CFMN	Mean	6.274E-03	6.274E-04	2.85E-05	1.34E-10	1.00	1.00	2.133E-02	3.213E+00	6.888E-01	0.057	0.00
2	9	Z	CFMN	Median	7.733E-05	7.733E-06	1.22E-03	5.72E-09	1.00	1.00	1.689E-02	2.807E+00	6.437E-01	0.056	0.00
1	10	D	TRW	Mean	1.856E-02	1.856E-03	2.04E-04	9.57E-10	1.00	1.00	2.682E-02	1.786E+00	4.402E-01	0.045	0.00
1	10	D	TRW	Median	2.122E-03	2.122E-04	7.76E-04	3.65E-09	1.00	1.00	1.114E-02	1.618E+00	3.820E-01	0.021	0.00
10-13	0	D	FAULTS	Mean	1.000E-07	1.000E-07	3.60E-06	1.69E-11	1.00	1.00	8.050E-03	1.610E+00	3.780E-01	0.021	0.00
10-13	0	D	FAULTS	Median	1.000E-07	1.000E-07	3.60E-06	1.69E-11	1.00	1.00	8.050E-03	1.610E+00	3.780E-01	0.021	0.00

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Figure 12-28. Vertical layers (with 4.6° dip) showing saturation profile through repository region.

Table 12-11. Well Data Used for STAFF3D Conceptual Model Calibration •

Well Name	Nevada St. Coord (m)		Nearest Coordinate		Node @ Wat Tbl	Measured Head (m)	Average of 36 Vectors	Mean Vector	Median Vector
	Easting	Northing	X-Dir (m)	Y-Dir (m)					
B-1	172,640	233,250	4,050	7,956	12,412	730.66	730.69	730.66	730.69
C-2**	173,620	230,690	4,900	5,556		0.00	730.00	729.96	730.02
C-3	173,600	230,710	4,900	5,556	15,764	730.10	729.98	729.96	730.02
G-1**	170,990	234,850	2,400	9,612		754.20	730.74	730.54	730.55
G-2	170,840	237,390	2,100	12,000	17,395	1,029.00	1,028.96	1,028.98	1,028.90
G-3	170,230	229,450	1,500	4,000	5,594	730.56	730.02	729.99	730.04
G-4**	171,627	233,418	3,000	8,184		0.00	730.66	730.53	730.55
H-1	171,420	234,770	2,700	9,612	9,001	730.95	730.53	730.51	730.54
H-3	170,220	230,590	1,500	5,556	4,730	731.72	730.18	730.15	730.19
H-4	171,880	232,150	3,300	6,776	10,328	730.33	730.40	730.37	730.41
H-5	170,360	233,670	1,800	8,412	6,027	775.47	775.86	775.86	775.86
H-6	168,880	232,650	300	7,356	3,998	775.96	775.86	775.86	775.86
J-13	176,680	228,360	8,000	3,000	17,523	728.45	728.63	728.63	728.63
P-1	174,190	230,480	5,700	5,000	16,657	730.00	729.64	729.61	729.67
WT-1	171,830	229,800	3,150	5,000	10,219	730.40	730.03	730.01	730.06
WT-10	168,650	228,230	0	3,000	3,727	775.92	775.86	775.86	775.86
WT-11	170,190	225,270	1,500	0	5,513	730.72	730.62	730.62	730.62
WT-12	172,820	225,470	4,200	0	12,872	729.52	729.69	729.69	729.69
WT-13	176,400	230,650	8,000	5,556	17,604	728.98	728.92	728.92	728.92
WT-14	175,320	232,150	6,850	6,776	17,684	729.71	729.83	729.81	729.88
WT-15	176,720	233,510	8,000	8,184	17,955	729.24	729.21	729.21	729.21
WT-16	173,860	236,040	5,300	10,812	17,358	738.32	738.32	738.29	738.39
WT-17	172,580	228,120	3,900	3,000	17,514	729.64	729.66	729.63	729.71

Table 12-11. Well Data Used for STAFF3D Conceptual Model Calibration (Continued)*

Well Name	Nevada St. Coord (m)		Nearest Coordinate		Node @ Wat Tbl	Measured Head (m)	Average of 36 Vectors	Mean Vector	Median Vector
	Easting	Northing	X-Dir (m)	Y-Dir (m)					
WT-18	172,170	235,050	3,600	9,612	11,761	730.80	730.44	730.42	730.44
WT-2	171,270	231,850	2,550	6,556	8,460	730.71	730.32	730.29	730.34
WT-3	174,770	227,380	5,700	1,500	16,576	729.57	729.16	729.15	729.19
WT-4	173,140	234,240	4,400	9,012	13,521	730.70	730.53	730.51	730.53
WT-6	172,070	237,920	3,450	13,000	18,348	1,035.10	1,035.10	1,035.10	1,035.10
WT-7	168,830	230,300	300	5,000	3,782	775.70	775.86	775.86	775.86
Average Absolute Difference from Measured Head=							0.21	0.22	0.22

* Model results are taken 100 years into the simulation.

** Head values not included in model calibration.

colation model described in Chapter 5.4, and imposed on the flow field as Neumann boundary conditions along the top plane of nodes. The "focus factor" used in the unsaturated zone model to simulate an enhanced flow region above the repository was not included in this saturated zone model

Model Flow Calibration: Initial and Boundary Conditions. An iterative process was used to calibrate model results to measured well data. First, values for fracture and matrix conductivities in the fault regions were assumed. Next, fixed head (Dirichlet) boundary conditions were derived by guessing a value for the northeast and southeast corners of the grid, and linearly interpolating Dirichlet conditions for the north, east, and south grid boundaries using these values and edge well values. The west grid boundary remained at a constant head of 775.86 m, which is the average head of wells WT-10, WT-7, and H-6. An initial condition of 730.5 m was assumed for all interior nodes in the mesh. The model was then allowed to run under dual porosity, steady-state conditions using the mean flow properties of the sampled parameters and a constant percolation of 0.5 mm/yr. The resulting values for head were compared to measured well data. If the match was poor, new values for fault conductivities and/or Dirichlet boundary conditions were assumed, and the procedure repeated. A reasonable match to measured well data was achieved, with an average error in head of 0.22 m (Table 12-11). Because the main objective of this model is to evaluate flow and transport in the saturated zone, a simple Brooks-Corey model was used ($n = 1$, or $K_{rw} = S_{weff}$) for the STAFF3D unsaturated zone relative permeability flow behavior in the fractures. STAFF3D neglects unsaturated matrix flow in its dual-porosity formulation, hence the capillary pressure behavior in the fractures was set equal to those in the matrix by using the same Van Genuchten parameters for capillary pressure. Doing so forced flow equilibrium between the fractures and matrix so that velocity fields could be obtained that were comparative with the unsaturated zone model. When a reasonable match with measured well data was achieved, 36 models were created, each representing a different sample set of flow parameters. The models representing the mean and median values of the sample set were run for 100,000 yr. Figure 12-29 shows piezometric head contours for the STAFF3D solution for the mean run. Figure 12-30 depicts the Darcy velocity fields generated from the flow results at the maximum percolation for the mean run. The Darcy velocities range from 10^{-8} to 10^{-10} m/s in the saturated layers below the repository, generally flowing north to south, then curving east beyond the 2,400-m release boundary.

12.4.3 STAFF3D Transport Model

Transport Properties. The transport parameters and radionuclide inventory used in the transport runs are presented in Table 12-12. The free-water diffusion and tortuosities used for all 36 models are the mean values reported in Chapters 9 and 11 of TSPA-1993 (Wilson et al., 1994). STAFF3D requires material-dependent chemical retardations as input to the transport model, hence the sorption coefficients (K_d) were converted to retardations by the following relationship:

$$R = 1 + (\rho_{bulk} * K_d) / (\phi * S_w), \text{ where } S_w = 1.0.$$

The material regions were subdivided into three main rock types: devitrified (D), vitrified (V), and zeolitic (Z), each with a different range of sorption coefficients for each isotope. For this analysis, the matrix sorption coefficients for Pu (devitrified rock type), U and Se (zeolitic rock type), and Pa and Np (devitrified and zeolitic rock types) were sampled, or varied, over the 36 sets. The vitrified rock sorption coefficients were set equal to the devitrified K_d s for all isotopes except Pa and Np, which were set to one-fourth of the devitrified value. Iodine and technetium were not retarded in the matrix ($K_d = 0$). Retardations for transport in the fractures were set to 1.0 ($K_d = 0$) for all isotopes and rock types. The sample ranges for the sorption coefficients were taken from TSPA-1993. The transport properties and inventory used for the STAFF3D saturated zone transport models are identical to those used in the NUTS calculations, except for longitudinal and transverse dispersivities. Longitudinal dispersivity for each of the 36 sets was determined by multiplying a uniformly sampled "dispersion fraction" times the model's transport distance. This distance was 300 m and 5000 m for the NUTS and STAFF3D models, respectively. The dispersion fraction was varied from 0.05 to 0.20; therefore, longitudinal dispersivity for the NUTS models ranged from 15 m to 60 m, and from 250 m to 1000 m for the STAFF3D models. Transverse dispersivity was set to one-tenth of the longitudinal dispersivity.

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Figure 12-29. Three-dimensional grid showing STAFF3D pressure head contours for horizontal mean saturated zone flow solution at 10,000 yr (z dimension is 5x magnification.)

(a) 2.4 km Boundary at 50,000 yr

(b) Entire Mesh at 50,000 yr

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Figure 12-30. Darcy velocity vectors for horizontal mean run at maximum rainfall infiltration.

Table 12-12. Transport Parameters and Radionuclide Inventory Used in STAFF3D Transport

Transport Parameters				Matrix Retardations:										Fracture Retard. All Nucl.
Mat.	Unit	Rock Type	Material Name	Vector	Bulk Density (Kg/m^3)	Matrix Porosity	Longitudinal Dispersion Matrix & Frac	Transverse Dispersion Matrix & Frac	[1+(Bulk Dens * Kd)/(Porosity * Sw). Sw = 1]				I & TC	
									U & SE	PU	PA & NP			
9	3	D	TSWC	Mean	2,258	0.139	625.0	62.5	41.61	1,625.46	33.49	1.00	1.00	
9	3	D	TSWC	Median	2,258	0.134	625.0	62.5	43.25	1,648.85	24.35	1.00	1.00	
8	4	V	TSW3	Mean	2,308	0.065	625.0	62.5	89.77	3,551.77	18.75	1.00	1.00	
8	4	V	TSW3	Median	2,318	0.055	625.0	62.5	107.19	4,142.51	15.67	1.00	1.00	
7	5	V	CHNV	Mean	1,838	0.331	625.0	62.5	14.88	556.29	3.78	1.00	1.00	
7	5	V	CHNV	Median	1,816	0.336	625.0	62.5	14.52	528.36	2.87	1.00	1.00	
6	6	Z	CHNZ	Mean	1,746	0.306	625.0	62.5	58.06	229.24	23.82	1.00	1.00	
6	6	Z	CHNZ	Median	1,743	0.306	625.0	62.5	55.74	223.51	16.74	1.00	1.00	
5	7	D	PPW	Mean	1,993	0.292	625.0	62.5	18.06	683.53	14.65	1.00	1.00	
5	7	D	PPW	Median	1,934	0.296	625.0	62.5	17.31	637.26	10.02	1.00	1.00	
4	9	Z	CFUN	Mean	2,021	0.261	625.0	62.5	78.43	310.73	31.97	1.00	1.00	
4	9	Z	CFUN	Median	2,037	0.257	625.0	62.5	77.12	310.43	22.89	1.00	1.00	
3	8	D	BFW	Mean	2,260	0.165	625.0	62.5	35.24	1,370.70	28.39	1.00	1.00	
3	8	D	BFW	Median	2,282	0.181	625.0	62.5	32.46	1,227.89	18.39	1.00	1.00	
2	9	Z	CFMN	Mean	2,021	0.261	625.0	62.5	78.43	310.73	31.97	1.00	1.00	
2	9	Z	CFMN	Median	2,037	0.257	625.0	62.5	77.12	310.43	22.89	1.00	1.00	
1	10	D	TRW	Mean	2,185	0.191	625.0	62.5	29.60	1,144.98	23.88	1.00	1.00	
1	10	D	TRW	Median	2,193	0.200	625.0	62.5	28.46	1,072.08	16.18	1.00	1.00	
10-13	0	D	FAULTS	Mean	2,366	0.087	625.0	62.5	68.99	2,720.54	55.39	1.00	1.00	
10-13	0	D	FAULTS	Median	2,366	0.087	625.0	62.5	68.99	2,652.72	38.58	1.00	1.00	

Table 12-12. Transport Parameters and Radionuclide Inventory Used in STAFF3D Transport (Continued)

INVENTORY for Aqueous Transport in Aquifer (Carbon 14 included for completeness)										*Sorption Coefficients (Kd) m ³ /kg				
Indx	Ele.	Atomic Mass	Half-Life (years)	Half-Life (sec)	Lambda 1/s	Activity Curie/kg	Parent Index	Free-Wat. Diffusion	Matrix Tortuosity	Fracture Tortuosity	Type D Mean	Type D Median	Type Z Mean	Type Z Median
1	U	238	4.47E+09	1.41E+17	4.915E-18	3.361E-04	0	1.00E-09	0.10	1.00	0.0025	0.0025	0.0100	0.0096
2	U	234	2.45E+05	7.72E+12	8.982E-14	6.247E+00	1	1.00E-09	0.10	1.00	0.0025	0.0025	0.0100	0.0096
3	PU	239	2.41E+04	7.59E+11	9.127E-13	6.216E+01	0	1.00E-09	0.10	1.00	0.1000	0.0975	0.0400	0.0391
4	U	235	7.04E+08	2.22E+16	3.120E-17	2.161E-03	3	1.00E-09	0.10	1.00	0.0025	0.0025	0.0100	0.0096
5	PA	231	3.28E+04	1.03E+12	6.701E-13	4.722E+01	4	1.00E-09	0.10	1.00	0.0020	0.0014	0.0040	0.0028
6	NP	237	2.14E+06	6.75E+13	1.026E-14	7.047E-01	0	1.00E-09	0.10	1.00	0.0020	0.0014	0.0040	0.0028
7	U	233	1.59E+05	5.00E+12	1.386E-13	9.678E+00	6	1.00E-09	0.10	1.00	0.0025	0.0025	0.0100	0.0096
8	I	129	1.57E+07	4.95E+14	1.399E-15	1.765E-01	0	1.00E-09	0.10	1.00	0.0000	0.0000	0.0000	0.0000
9	TC	99	2.13E+05	6.72E+12	1.031E-13	1.695E+01	0	1.00E-09	0.10	1.00	0.0000	0.0000	0.0000	0.0000
10	SE	79	6.50E+04	2.05E+12	3.381E-13	6.965E+01	0	1.00E-09	0.10	1.00	0.0025	0.0025	0.0100	0.0096
11	U	236	2.34E+07	7.39E+14	9.381E-16	6.469E-02	0	1.00E-09	0.10	1.00	0.0025	0.0025	0.0100	0.0096
0	C	14	5.73E+03	1.81E+11	3.833E-12	4.456E+03	0	1.00E-09	0.10	1.00	N/A	N/A	N/A	N/A

* kd's for vitric rocks (type V) = kdD (for U, PU, I, TC, SE). kdV = 0.25 * kdD (for PA & NP).

Initial and Boundary Conditions, Coupling to NUTS Output. All initial concentrations (time zero) were set to zero. The NUTS unsaturated zone transport results were used as a time-dependent flux source to the STAFF3D model. The BRAGFLO_T/NUTS mesh used for unsaturated zone flow and transport is a two-dimensional, axisymmetric finite-difference model, which is completely different from the three-dimensional finite-element mesh used in STAFF3D. Hence, the radionuclide concentrations from NUTS were decoupled from the grid geometry by converting them to the mass flux, in kg/s, that crosses the upstream grid-block interface for both the x and y directions at each time step. The downward (negative z direction) mass fluxes for each radionuclide were summed over the element rows at a specified vertical distance representing the water table within the BRAGFLO_T/NUTS grid. These mass fluxes were then redistributed as time-dependent flux boundary conditions at the nodal points representing a similar surface water table area within the STAFF3D grid. It should be noted that the elements chosen to represent the BRAGFLO_T water table for STAFF3D coupling were approximately 100 m above the physical water table (100% water-saturated elements), or, at the top of the CHnz unit instead of the bottom. This location was selected to avoid the slight numerical instabilities encountered at the water table due to capillary pressure and phase effects (see Sections 12.1.1 and 12.1.2), as well as to account for any possible rise in the water table. STAFF3D creates a lookup table of time-dependent mass fluxes for each radionuclide to interpolate for every STAFF3D time step throughout the transport calculation. Two sets of 36 STAFF3D models were created, representing both the horizontal and vertical waste emplacement schemes. A zero concentration gradient boundary condition was assumed at all external grid boundaries, which allows advection at the boundaries, but not diffusion. Solute is allowed to flow out of, but not into, the grid.

Dual-Porosity Transport Behavior. For dual porosity, STAFF3D calculates advective/dispersive transport in the fractures with matrix diffusion. The Darcy velocity components needed for the advective transport in the fracture are read in from the STAFF3D flow solution for each of the 36 models. Of the 11 radionuclides transported, only ^{99}Tc and ^{129}I travelled any significant distance from the source nodes (at the top of the water table) during the 10,000-yr regulatory period. This result is to be expected, as these are the only two isotopes with zero chemical sorption onto the matrix rock surface (retardation equal to one). The nine remaining isotopes considered for aqueous transport are controlled by varying degrees of chemical retardation, and therefore do not reach the water table in significant quantities for the first 10,000 yr. Technetium has the highest releases (in kilograms) to the water table and beyond for all 36 runs for horizontal and vertical emplacement. Figures 12-31 and 12-32 show concentration contours of ^{99}Tc for the BFW and CHnz units at 10,000, 50,000, and 100,000 yr. The effect of the rainfall percolation model can be seen, as the technetium has been swept out of the shallower CHnz unit (Figure 12-32) through the bottom of the layer and out the sides of the grid. The deeper BFW unit retains more of the isotope at later times, but has only small amounts present ($<10^{-12} \text{ kg/m}^3$) through the first 10,000 yr (Figure 12-31). At later times (after 10,000 yr), uranium and neptunium reach the water table in more significant amounts. Figure 12-33 shows the spread of contamination of ^{233}U over time and is typical of the other uranium isotopes since they are controlled by the same sorption coefficients. The amount of each uranium isotope that reaches the water table becomes a function of the volumes escaping the waste emplacement packages, which is controlled by the uranium inventory and parameters affecting the source term model. Generally, ^{234}U had the most releases out of the repository compared to the other uranium isotopes. Neptunium becomes the dominant radionuclide released to the water table after 10,000 yr for the mean and median runs, which is due to its high inventory (including the fathers in its decay chain) and relatively low sorption coefficients. Figure 12-34 shows that ^{237}Np concentrations in the water table are still increasing at 100,000 yr. The ^{237}Np contaminant plume has permeated the mesh, reaching the deeper geologic units (Figure 12-35) as well as the shallower units (Figure 12-36) by 100,000 yr. It should be noted that the solute concentrations within the water table for all the isotopes are quite low, ranging from 10^{-6} to 10^{-12} kg/m^3 for the 10,000-yr regulatory period.

12.4.4 Intermediate Results for Saturated Zone Transport

Figure 12-37 is a CCDF that shows the amount of releases for the saturated model source input that reach the water table over 10,000 yr. Even if downward releases were considered a compliance measure (which they are not), Figure 12-37 shows that the entire amount of releases entering the water table comply with 40 CFR 191 prior to saturated zone transport for both horizontal and vertical waste emplacements. Figures 12-38 and 12-39 illustrate how the geologic barrier, as described by the BRAGFLO_T/NUTS conceptual models, greatly impedes releases to the environment. A significant portion of the radioactivity released from the waste parcels escapes from the repository (engi-

12. Complex Consequence Modeling

(a) 10,000 yr

(b) 50,000 yr

(c) 100,000 yr

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Figure 12-31. Concentrations of ^{99}Tc (kg/m^3) at various times within the BFW unit for the horizontal mean run.

(a) 10,000 yr

(b) 50,000 yr

(c) 100,000 yr

TRI-6342-5081-0

Figure 12-32. Concentrations of ^{99}Tc (kg/m^3) at various times within the CHNz unit for the horizontal mean run.

(a) 10,000 yr

(b) 50,000 yr

(c) 100,000 yr

TRI-6342-5082-0

Figure 12-33. Concentrations of ^{233}U (kg/m^3) at various times within the CHNz unit for the horizontal mean run.

(a) 10,000 yr

(b) 50,000 yr

(c) 100,000 yr

TRI-6342-5083-0

Figure 12-34. Concentrations of ^{237}Np (kg/m^3) at various times within the CHNz unit for the horizontal mean run.

(a) CFMn

(b) BFw

(c) CFUn

TRI-6342-5084-0

Figure 12-35. Concentrations of ^{237}Np (kg/m^3) at 100,000 yr within the CFMn, BFw, and CFUn units for the horizontal mean run.

(a) CHnv

(b) TSww

(c) TSww

TRI-6342-5085-0

Figure 12-36. Concentrations of ^{237}Np (kg/m^3) at 100,000 yr within the CHnv, TSww, and TSw units for the horizontal mean run.

Figure 12-37. CCDF showing downward releases reaching the water table for the 36 horizontal emplacement waste parcels, and the 36 vertical waste emplacement parcels.

(a) Leaving the Waste Parcels

(b) Leaving the Repository

(c) Entering the Water Table

TRI-6342-3608-0

Figure 12-38. Time history plots (36 vectors) showing total activity of all radionuclides at various release locations for aqueous transport: horizontal emplacement.

12. Complex Consequence Modeling

(a) Leaving the Waste Parcels

(b) Leaving the Repository

(c) Entering the Water Table

TRI-6342-3610-0

Figure 12-39. Time history (36 vectors) plots showing total activity of all radionuclides at various release locations for aqueous transport: vertical emplacement.

1 neered barrier system as modeled for the 1994 PA), yet very little of those releases reach the water table after
2 10,000 yr. Apparently most releases are confined in the unsaturated region between the repository and the water
3 table.
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6 Similarly the geologic barrier modeled for the saturated zone transport (STAFF3D) tends to contain releases in
7 the water table as depicted in Figures 12-40 and 12-41. Of the 36 consequences modeled, very few result in contam-
8 ination reaching the 2400-m saturated zone boundary and those that do total less than one-tenth of a curie (Figures
9 12-40a and 12-41a). The only radionuclides that reach the boundary after 10,000 yr are technetium and iodine, with
10 cumulative masses totalling less than 0.01 kg for both horizontal and vertical waste emplacements (Figures 12-40b,c
11 and 12-41b,c). As expected, solute releases to the environment are directly related to the volume of water flowing
12 through the repository. The transport properties (sorption coefficients and dispersivities) appear to have less of an
13 influence on releases. Figure 12-42a shows a scatterplot of releases to the water table versus dispersion multiplier
14 (i.e., fraction multiplied by 300 m to obtain longitudinal dispersivity in the NUTS models). As can be seen, no dis-
15 cernible correlation exists, with high releases seen for both large and small dispersivities. When releases are plotted
16 against liquid flow through the repository (Figures 12-42b), a definite pattern develops with the higher flows resulting
17 in more radioactivity to the water table. The importance of chemical retardation is apparent since the isotopes with
18 non-zero sorption coefficients do not reach the water table in 10,000 yr, even at the highest liquid flow rates. The
19 degree of chemical retardation appears to become more influential for liquid releases over longer times.
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25 12.5 Summary of Information Gathered from Complex PA

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28 Table 12-13 provides a summary of information gathered about the repository, geologic barrier, and agents acting
29 on the tuff disposal system.
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(a) Total Radionuclides for Aqueous Transport

(b) ^{99}Tc (c) ^{129}I

TRI-6342-3609-0

Figure 12-40. Releases at the 2,400 m boundary: horizontal emplacement.

(a) Total Radionuclides for Aqueous Transport

(b) ^{99}Tc (c) ^{129}I

TRI-6342-3611-0

Figure 12-41. Releases at the 2,400 m boundary: vertical emplacement.

TRI-6342-5087-0

(a)

TRI-6342-5088-0

(b)

Figure 12-42. Total radioactivity reaching the water table at 10,000 yr (a) vs dispersivity multiplier, and (b) vs cumulative water flow through the bottom of the repository (negative indicates downward flow).

Table 12-13. Summary of Information Gathered from Complex PA

Repository

1. The thermal power density and its influence on local temperatures in the repository has a very strong effect on the behavior of liquid and gas flow through and around the repository (Figure ES-9).
2. The 65% water saturation in the horizontal emplacement scheme in the tuff matrix is sufficient to keep temperatures in computational grid blocks below 100°C as water vaporizes. Thus maximum local temperatures in the repository are substantially lower than those calculated when only heat conduction and radioactive heat transfer are considered.
 - In the horizontal emplacement scheme, repository temperatures increase from an initial value of 26°C to a maximum value of about 93°C (thus, no dry-out zone), and then fall slowly. The peak temperature is reached at the center of the repository, about 30 yr after waste disposal.
 - In the vertical emplacement scheme, the maximum repository temperature is about 25°C lower than for horizontal emplacement.
 - When only heat conduction and radioactive heat transfer are considered, the maximum repository temperature for horizontal emplacement is about 134°C.
3. Between 0 and 500 yr, gas flow is dominated by vaporization of water in the repository, movement out in all directions in the highly conductive fracture network, and then condensation all around the repository.
 - Because of water vaporization, the air mass percentage drops from an initial value of 92% to 30%. Assuming the mole percentage of oxygen in air is 21%, the oxygen percentage in the gas phase drops to 7% by mass and 4.4% by moles. Because anoxic corrosion rates are generally lower than oxic corrosion rates, the lack of oxygen could counteract somewhat the greatly increased corrosion rate from the temperature increase during the first 500 yr (period dominated by local gas movement).
 - This vaporization process produces a rise in gas pressure. In the horizontal and vertical emplacement schemes, the pressure rises to a maximum of 0.1044 and 0.1042 MPa, respectively. The corresponding drop in liquid pressure draws water towards the repository. In the horizontal emplacement scheme, water is drawn from as far away as the water table, located 300 m below the repository.
4. After 1000 yr, gas flow is dominated by the regional circulation of gas caused from the heating of the area around the repository; the regional circulation does not diminish substantially over the next 9000 yr.
 - General heat conduction through the rock matrix adequately predicts the general temperature profile on a regional scale after 1000 yr.
 - The travel time to the surface of gas originating in the repository is fastest once the regional gas flow circulation pattern has been established.
5. Gas consumption from oxic corrosion of the containers had little influence on the flow of gas.

Geologic Barrier

6. Inclusion of sorption of radionuclides on tuff within the unsaturated and saturated zones greatly diminished the release of radionuclides.
 - The only radionuclides to reach the water table in 10,000 yr were minute amounts of uranium and neptunium, because of their high initial quantity and only moderate sorption, and larger amounts of radionuclides that are not readily sorbed (^{129}I , and ^{99}Tc).
 - No radionuclides in meaningful quantities entering the saturated zone reached the 2.4-km boundary in 10,000 yr.
7. The reduced solubility assumed for uranium in water saturated with silica and the moderate sorption assumed greatly diminished the amount of uranium reaching the water table. In addition, sorption of plutonium by tuff inhibited its release from the waste disposal region and prevented plutonium from even reaching the water table.
8. Between 10,000 and 50,000 yr, additional amounts of uranium (^{233}U , ^{234}U) and large amounts of neptunium (^{233}Np) reach the water table.

Table 12-13. Summary of Information Gathered from Complex PA (Continued)

9. By 100,000 yr, results from the deterministic run using mean values (horizontal emplacement) show that about 0.156 kg of ^{237}Np , 0.195 kg of ^{129}I , and 3.37 kg of ^{99}Tc (about 57 curies total), have left the 2.4-km boundary.

Agents Acting on the Tuff Disposal System

10. Climatic change and its assumed direct influence on water infiltration had only a minor influence on the flow of water to the water table in the 10,000-yr simulation* in the Complex PA using a two-dimensional model.
- For horizontal emplacement, many simulations showed cumulative flow from the water table to the repository as the result of lower liquid pressures as water is vaporized around the repository in the first 1000 yr.
 - All particles released at the surface to track percolating water were trapped in the high porosity PTn layer above the repository, which suggests that little flow from the surface passes into the TSw layer until the saturation level of the matrix is raised enough to allow some flow in the fractures.
11. Potential concentration of infiltration or percolation above the repository is influential in getting water to the repository after about 3000 yr by changing the flow regime from matrix flow to fracture flow in the Complex PA.
12. In contrast to the Complex PA, the three parameters for climatic change (see Table ES-11) were the most important model parameters in the Simple PA.

* 40 CFR 191 clearly stated in the preamble to the 1985 promulgation of the regulation that a time period was purposely selected by the EPA such that changes occurring on a geologic time scale would not affect the compliance evaluation.

13. Simplified Consequence Modeling

M. L. Wilson, M. S. Tierney, J. W. Berglund, and A. H. Treadway

In the Simple PA, the approach to evaluating the potential consequences of release from a tuff disposal system is similar to the Sandia performance assessments of the Yucca Mountain Project (Barnard et al., 1992; Wilson et al., 1994). In these assessments, processes such as heat transport and fluid transport were not coupled. The Simple PA uses one major code from the previous assessment of Yucca Mountain, TOSPAC (Dudley et al., 1989).

Four models are used in the Simple PA to evaluate five conditions: (1) heat conduction, (2) water percolation, (3) radionuclide transport in percolating water in the unsaturated zone, (4) gaseous ^{14}C transport, and (5) radionuclide transport in the saturated zone. (Section 7.5 contains a discussion regarding how these four models are linked to the overall modeling system.) The discussions below include descriptions of the conceptual models, mathematical implementations, and applied models for the Simple PA. (The numerical solution of the mathematical model is generally not included.) Results for each applied model are provided, but the summary measures of these results, which are expressed primarily as complementary cumulative distribution functions (CCDFs) are presented in Chapter 15, "Performance Measures, Sensitivity Analysis, and Recommendations."

13.1 Heat Conduction and Radiative Heat Transfer (J. W. Berglund)

For the Simple PA, thermal conduction calculations were performed to generate heat output values for individual waste parcel types. The data were used directly by the source term submodel, USATCONC (Chapter 11).

13.1.1 Code Descriptions for Thermal Conduction Calculations

For the Simple PA, two thermal conduction codes—CONRAD and SUMQ_3D—were used to determine time-dependent temperature distributions near a container and within the repository. As described in Section 12.2 for the Complex PA, CONRAD, a modified version of the heat-conduction code, COND_1D (used in the 1993 PA), was used to determine near-field temperatures. CONRAD treats thermal conduction in an axisymmetric geometry and allows for radiation heat transport across an air gap. For the Simple PA, these near-field temperatures were corrected by adding the temperature of the overall repository, which was obtained from the SUMQ_3D computations. (For the Complex PA (Chapter 12), CONRAD results were combined with temperatures computed by BRAGFLO_T. Specific details about BRAGFLO_T and CONRAD are provided in Sections 12.1 and 12.2, respectively.)

For the Simple PA, SUMQ_3D was used to compute the far-field, transient thermal response within the repository. SUMQ_3D generates time-dependent temperatures for all containers in the repository. SUMQ_3D is designed to determine the temperature at any point and at any time within an arbitrary array of decaying thermal line sources of finite length. The code is based on the superposition of a large number of decaying point source solutions in an infinite medium.

The governing equations for SUMQ_3D are based upon analytical work discussed in Carslaw and Jaeger (1959). The temperature change at any point in a field away from a constant thermal source and at any time, assuming constant conductivity and diffusivity, is governed by the equation:

$$\Delta T = \frac{\bar{q}}{4\pi Kr} \operatorname{erfc} \left[\frac{r}{\sqrt{4kt}} \right] \quad (13-1)$$

where

ΔT	=	temperature change,
$\bar{q}$	=	source strength,
K	=	thermal conductivity,
r	=	radius from source,

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k = thermal diffusivity,
t = time.

When the source decays with time, the governing equations must be written in integral form as

$$\Delta T = \frac{k}{4K(\pi k)^{\frac{3}{2}}} \int_0^{\infty} \frac{q}{\sqrt{t}} \left(t - \frac{1}{\tau^2} \right) \exp\left(-\frac{r^2 \tau^2}{4k} \right) d\tau \quad (13-2)$$

To model a constant thermal source, the solutions to an array of point sources (Equation 13-1) are configured to approximate a field of containers of finite length and summed to determine the temperature change at any point and at any time. Typically, a container can be represented by 50 point sources. SUMQ_3D can model many thousands of containers, although fewer can be used to determine the temperature change at a particular point. Thus, for a 1000-container array, Equation 13-1 would be solved 50,000 times and the results summed to obtain the temperature at a single point. When thermal decay is taken into account, a similar process is used with Equation 13-2, which must be integrated numerically.

13.1.2 Calculations for Repository with Horizontal Waste Emplacement

The calculations for the repository with horizontal waste emplacement assumed that containers were placed end to end in waste disposal rooms (see Figure 13-1). The number of rooms and center-to-center spacing between waste disposal rooms was varied to maintain a constant initial thermal power and power density (see Table 13-1).^{*} Each room was 426 m long. All containers were circular in cross-section and separated from the tuff by a 1.255-m air gap.

The waste disposal rooms were each assumed to be a 426-m-long linear heat source. The thermal power from each waste disposal room equals 1/N of the repository total, where N represents the number of waste disposal rooms (see Figure 13-1). The thermal conduction and radiation properties are the same as those provided in Chapter 12, Table 12-1.

SUMQ_3D was used to compute the thermal response between containers out to 10,000 yr. Local transient temperatures were computed for each waste type with CONRAD. The total temperatures within and near each container were then obtained by adding the SUMQ_3D results to the temperature changes calculated by CONRAD. Figure 13-2 provides the temperature response for the canister center at the center and edge of the repository with horizontal emplacement. Figure 13-3 shows the temperature at the repository edge and the TS/CH interface for the horizontal emplacement. Figure 13-4 shows the temperature at the repository center for horizontal and vertical emplacement.

13.1.3 Calculations for Repository with Vertical Waste Emplacement

The calculations for the repository with vertical waste emplacement assumed that a single type of waste was placed in the repository, 489 waste parcels were emplaced in boreholes in each of the waste disposal rooms, and the boreholes were arranged in a 2.6-m spacing hexagonal pattern (Figure 13-5). The number of rooms and the center-to-center spacing between waste disposal rooms was varied to maintain a constant thermal power and power density (see Table 13-1).^{*} The waste disposal rooms were 426 m long. All containers were assumed to be circular in cross-section; equivalent round cross-sections based on area were used for non-round cross-sections. An air gap of 0.025 m between the container and tuff was assumed.

^{*} Note that the thermal power computed for the total number of containers of INEL calcine high-level waste as borosilicate glass (WP 110, WP 210) is lower than the other waste types. INEL calcine is relatively cool because of reprocessing and requires a large number of containers when packaged as borosilicate glass, so an initial thermal power equivalent to the other waste types could not be modeled.

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Figure 13-1. Horizontal emplacement repository.

Table 13-1. Repository Design Summary for Simple PA

Waste	Container ID#	No. of Containers used in Simple PA	Power Computed from Total No. of Containers (W)	Computed Design-Basis APD (W/m ²)	Disposal Region Area (m ²)	Number of Waste Disposal Rooms
Horizontal Orientation						
Graphite SNF	101	20072	3.4323×10^6	3.7578	4.598×10^5	251
N-Reactor	102	2106	3.4328×10^6	23.192	4.946×10^4	27
Shippingport SNF	103	1700	3.4340×10^6	23.192	4.030×10^4	22
ATR (HEU) SNF	104	816	3.4354×10^6	23.192	2.015×10^4	11
PWR (LEU) SNF	105	1575	3.4335×10^6	23.192	3.847×10^4	21
INEL Calcine G/C HLW	106	114408	3.4322×10^6	0.94274	1.839×10^6	1004
DOE Savannah HLW	107	2617	3.4335×10^6	23.192	4.213×10^4	23
DOE Hanford HLW	108	2195	3.4330×10^6	23.192	3.664×10^4	20
DOE West Valley HLW	109	5838	3.4327×10^6	18.456	9.525×10^4	52
INEL Calcine B/G HLW	110	347017	2.7761×10^6	0.25141	5.578×10^6	3045
INEL Calcine Loose HLW	111	100768	3.4342×10^6	1.0703	1.619×10^6	884
Vertical Orientation						
Graphite SNF	201	135057	3.4304×10^6	2.4609	8.992×10^5	277
N-Reactor	202	14075	3.4343×10^6	14.156	9.414×10^4	29
Shippingport SNF	203	10191	3.4344×10^6	14.156	6.817×10^4	21
ATR (HEU) SNF	204	5753	3.4345×10^6	14.156	3.895×10^4	12
PWR (LEU) SNF	205	11008	3.4345×10^6	14.156	7.466×10^4	23
INEL Calcine G/C HLW	206	457895	3.4342×10^6	0.72595	3.042×10^6	937
DOE Savannah HLW	207	10471	3.4345×10^6	14.156	7.141×10^4	22
DOE Hanford HLW	208	8784	3.4345×10^6	14.156	5.843×10^4	18
DOE West Valley HLW	209	23362	3.4342×10^6	14.156	1.558×10^5	48
INEL Calcine B/G HLW	210	840103	1.680×10^6	0.19283	5.580×10^6	1719
INEL Calcine Loose HLW	211	403845	3.4408×10^6	0.82310	2.681×10^6	826

To achieve sufficient temperature detail near a container located at the center of the repository (and also at the repository edge), the middle three waste disposal rooms were modeled in detail. These three rooms included a total of 1467 containers (3×489), each modeled as 4.5-m-long linear heat sources. The thermal response was calculated for 11 waste types, corresponding to waste parcels 201 through 211.

The remaining waste disposal rooms (N-3) were assumed to be 426-m-long linear heat sources. The thermal power from each waste disposal room equals the total power of the 489 containers per room. The thermal conduction and radiation properties considered are the same as those provided in Chapter 12, Table 12-1.

(a)

(b)

(c)

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Figure 13-2. Temperature for horizontal emplacement at the (a) container center at the center of the repository, (b) container center at the edge of the repository, and (c) container wall at the center of the repository.

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Figure 13-3. Temperature at the (a) repository edge and (b) TS/CH interface for the horizontal emplacement.

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Figure 13-4. Temperature at repository center for (a) horizontal and (b) vertical emplacement.

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Figure 13-5. Thermal conduction modeling for repository with vertical waste emplacement.

Local transient temperatures were computed for each waste type with CONRAD. The total temperatures within and near each container were then obtained by adding the SUMQ_3D results to the temperature changes calculated by CONRAD. Figure 13-6 shows the combined results for temperature response at the canister center at the center and edge of the repository with vertical emplacement.

13.1.4 Computed Thermal Histories

For both vertical and horizontal emplacement, most temperature histories for the containers conform to a pattern of a rapid rise in temperature, followed by a gradual decrease in temperature out to 10,000 yr. The early, rapid rise in temperature (tens of years) is the result of local heating effects within the container. A second increase in temperature generally occurs later in time (hundreds of years) and is the result of the heating from all containers in the repository.

The peak temperatures achieved for the repositories modeled in the Simple PA are considerably higher than for the Complex PA, where the waste was disposed as a waste disposal group. The temperature histories for the Simple PA are also more sensitive to the rates of radionuclide decay for each type of waste parcel than the histories for the Complex PA, especially at late times (i.e., hundreds of years). Although the temperatures for the vertical emplacement are lower, the differences in areal power density (see Table 13-1) account for the differences in temperature between the horizontal emplacement (Figure 13-2) and the vertical (Figure 13-6).

13.2 Water Percolation in Unsaturated Zone (M. L. Wilson)

13.2.1 Conceptual/Mathematical Model

Coupling of Fracture and Matrix Flow (Composite-Porosity Model). The unsaturated zone in the tuff disposal system consists of about 600 m of stratified, fractured tuffs with several faults. The actual interaction of the fractures with the matrix is unknown. Like the Complex PA (described in Chapter 12), a composite-porosity model is used to represent flow, driven by gravity and capillary forces, in the fractured tuff. The major assumption of a composite-porosity model, which is a simplification of a dual-permeability model, is called the equilibrium assumption and is the close coupling of matrix and fracture flow such that pressure heads within both the matrix and fracture subdivisions of the tuff are equal at all times.

A corollary to the equilibrium assumption is that one of the major parameters of Darcy's law, hydraulic conductivity (K), can be described separately for the matrix and fractures, then combined in an area-weighted average. For example, Darcy's law in one dimension is expressed in the composite-porosity model as follows:

$$q = -K \left(\frac{\partial \Psi}{\partial z} + 1 \right) \quad (13-3)$$

$$\Rightarrow q = -\frac{A_m K_m + A_f K_f}{A_m + A_f} \left(\frac{\partial \Psi}{\partial z} + 1 \right), \quad (13-4)$$

where q is the groundwater flux or Darcy velocity (through the composite medium), Ψ is the pressure head (the same in the matrix and fractures for this model), z is the elevation A_m and A_f are the cross-sectional areas of the one-dimensional column for the matrix and fractures, respectively, and K_m and K_f are the hydraulic conductivities of the matrix and fractures, respectively. Given the solution for the pressure head and the assumption of pressure equilibrium between matrix and fractures, the flux in matrix and in fractures is given by

$$q_m = -K_m(\Psi) \left(\frac{\partial \Psi}{\partial z} + 1 \right), \quad (13-5)$$

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(a)

(b)

(c)

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Figure 13-6. Temperature for vertical emplacement at the (a) container center at the center of the repository, (b) container center at the edge of the repository, and (c) container wall at the center of the repository.

$$q_f = -K_f(\psi) \left(\frac{\partial \psi}{\partial z} + 1 \right). \quad (13-6)$$

The radionuclide-transport equations require moisture content and transport velocity in matrix and fractures. Moisture contents are determined directly from the characteristic curves (the functional relation between saturation and pressure head):

$$\theta_m = \phi_m S_m(\psi), \quad (13-7)$$

$$\theta_f = \phi_f S_f(\psi), \quad (13-8)$$

where θ denotes moisture content, ϕ denotes porosity, and S denotes liquid saturation. The effective transport velocity is given by percolation flux divided by moisture content:

$$v_m = q_m / \theta_m, \quad (13-9)$$

$$v_f = q_f / \theta_f. \quad (13-10)$$

For further discussion of the composite-porosity model, refer to Chapter 12 in this report, Peters and Klavetter (1988), and Dudley et al. (1989).

Unsaturated Fluid Flow (Steady State). In contrast to the Complex PA, the Simple PA does not track the flow of gas (such as air) and liquid (such as water). Instead, the mathematical formulation used in the Simple PA is Darcy's equation as written for the liquid flow component. The steady-state solution is obtained in the Simple PA.

13.2.2 Computational Model

Using Darcy's law and assuming a composite-porosity medium, liquid flow in the unsaturated zone is numerically implemented in TOSPAC (Dudley et al., 1989; Gauthier et al., 1992). When the pressure head is known, saturation and hydraulic conductivity are calculated from characteristic curves as described by van Genuchten (1980). Different characteristic curves are used for the matrix and the fractures so that water fluxes and velocities can be calculated for both. Also, for numerical stability, a derivative of Equation 13-4 is used so that the equation more closely resembles the conservation-of-mass formulation.

13.2.3 Applied Model

The description of the tuff medium, including its physical dimensions and hydrologic properties, is similar to that used in the Complex PA and described in Chapter 5, "Geologic Barrier." For purposes of the Simple PA, the unsaturated zone was represented by a vertical column with flow and transport in one dimension only, but with an area corresponding to the given repository area. The stratigraphy for the center of the repository was used for the vertical column and is shown in Figure 13-7. The repository was located with its top 1 m below the nominal floor of the waste disposal rooms and extending downward 5 m. This location is approximately correct for vertically emplaced canisters. Horizontally emplaced canisters would actually be located higher—above the drift floor—but for simplicity the same location was used for both vertical and horizontal cases.

As shown in Figure 13-7, the computational column started 18 m above the top of the repository (17 m above the nominal drift floor), rather than extending all the way to the ground surface. Aqueous transport took place only below the repository, so there was no need to include the upper part of the mountain in the calculational domain. (And in a one-dimensional flow calculation, the solution at a point depends only on points below it, since total flux, q , is constant.)

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Figure 13-7. Calculational mesh for Simple PA unsaturated-zone aqueous flow and transport.

Figure 13-7 also shows the computational mesh used for the unsaturated-zone flow and transport calculations. To minimize numerical dispersion, a maximum cell size of 1 m was used, with smaller cells at geologic-unit interfaces.

The column area depended on the number of waste disposal rooms used. The area for each case is given in Table 13-1.

Boundary conditions for the one-dimensional calculations were simply zero pressure head ($\psi = 0$) at the bottom boundary (the water table) and the sampled value of infiltration q at the top boundary. See Chapter 5 for a discussion of the infiltration values used.

13.2.4 Fluid Flow Results

Figures 13-8 through 13-10 show the flow solution for the case in which median values are used for all sampled parameters. The flow is high enough ($q = 2.6 \times 10^{-11}$ m/s, or 0.81 mm/yr) that the matrix is nearly saturated everywhere. However, the flow is still well below the amount that the fractures can handle, so the fractures are only slightly above their residual saturation. The CHnv unit has a much higher matrix saturated conductivity than the other units, and this is visible in the fact that the fracture velocity is much lower in that unit than in the other units (Figure 13-10). The reason for the lower fracture velocity is that significant fracture flow occurs in the composite-porosity model only if the percolation flux exceeds the matrix saturated conductivity.

One of the most important parameters that determines the amount of radioactivity release within 10,000 yr is the amount of water flow through the unsaturated zone, i.e., the percolation flux. In the Simple PA, the percolation flux is a constant for each simulation, and it is worth looking at the distribution of values. As described in Chapter 5, the value used for each simulation is a weighted average of the dry-climate and wet-climate infiltrations, with the dry-

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Figure 13-8. Flow solution for pressure head of water vs. elevation. Median values were used for all sampled parameters.

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Figure 13-9. Flow solution for matrix and fracture moisture contents vs. elevation. Median values were used for all sampled parameters.

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Figure 13-10. Flow solution for effective water velocity for transport vs. elevation. Median values were used for all sampled parameters.

climate infiltration weighted more heavily. The resultant distribution is shown in Figure 13-11. In that figure, it can be seen that most simulations have percolation flux below 1 mm/yr, but there is a long tail going up to 2.7 mm/yr.

13.2.5 Gas Flow in Unsaturated Zone (M. S. Tierney)

Releases of ^{14}C in the form of the gas $^{14}\text{CO}_2$ are expected to be important for spent-fuel repositories in the vadose zone (Barnard et al., 1992). Thermally driven air currents in the partially saturated overburden of these repositories can lead to transport of radionuclide-bearing gases or vapors to the atmosphere on time scales that are short compared to typical groundwater travel times. If the repository contains significant inventories of ^{14}C in the fuel pellet-cladding gaps, or as an activation product, and mobilization of carbon from these sources is relatively rapid on the regulatory time scale (10,000 yr), there is a potential for releases of radioactivity to the accessible environment that exceed limits set by 40 CFR 191 (Chapter 2). Assessing the magnitude of these gaseous releases requires mathematical models of thermally driven gas flows in vadose-zone repositories and the attendant transport of gas-phase radioactive elements in those gas flows.

Ross and coworkers have developed mathematical models of gas flow and $^{14}\text{CO}_2$ transport through the unsaturated zone of the Yucca Mountain repository site (Ross et al., 1992). Because they are computational intensive, we were not able to use these models directly in the present "Simple PA." Instead, we have made analytic fits to some results of the Ross et al. flow models that were calculated for the Yucca Mountain Project (Barnard et al., 1992; Wilson et al., 1994), and have employed the analytic representations of flow as input to a simplified calculation of gas-phase releases of ^{14}C to the accessible environment (Section 13.4). The essential features of the version of the Ross et al. model of gas flow used in the present study are described below.

The Ross et al. computer model, called TGIF, solves conservation equations of air volume and energy, coupled with Darcy's Law and the Ideal Gas Law, on a two-dimensional, finite-difference mesh that can represent various vertical cross-sections of the Yucca Mountain repository site (Figure 13-12). Principal assumptions of TGIF are

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Figure 13-11. Percolation probability density function and cumulative distribution function for 36 simulations.

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Figure 13-12. Finite-difference mesh for cross section N765000. Only heat conduction is modeled in the lower part of the mesh; heat and gas flow are modeled in the upper of the mesh (Ross et al., 1992).

- Flow and temperature profiles are steady.
- Thermodynamic equilibrium among air, water vapor, and water.
- The gas is saturated with water vapor.
- Changes in partial pressure of water vapor are accommodated by changes in gas composition, with the total pressure remaining nearly constant.
- Molecular diffusion resulting from gradients of water-vapor partial pressure has a negligible effect on gas flow.
- Porous matrix and fractures in the overburden are treated together as an equivalent porous medium.

The output of TGIF is a set of velocity fields defined on the fixed finite-difference mesh; each field corresponds to a fixed repository temperature and ratio of permeabilities of the nonwelded/welded tuff units. An example of such a velocity field is shown in Figure 13-13.

13.3 Aqueous Radionuclide Transport in Unsaturated Zone (M. L. Wilson)

The transport model used for this study is implemented in the TRANS module of the computer program TOSPAC; for a complete discussion of the model, see Dudley et al. (1989). The following is a general discussion of how the model represents transport, and the model assumptions that are significant to this study.

13.3.1 Liquid Phase Transport (M. L. Wilson)

TRANS is a one-dimensional dual-continuum model of solute transport, containing two generalized advection-dispersion differential equations. The equation for solute transport through a rock matrix is as follows:

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Figure 13-13. Path lines with the repository heated to 330 K and nonwelded/welded permeability ratio of 0.01 (0.1 in faulted area). Cross-section N762500. (Taken from Figure 6-14 of Ross et al., 1992).

$$\begin{aligned}
 \frac{\partial}{\partial t} (R_m^i \theta_m C_m^i) = & - \frac{\partial}{\partial z} \left(C_m^i q_m - \theta_m D_m^i \frac{\partial C_m^i}{\partial z} \right) & [\text{Advective and Dispersive Terms}] \\
 & - \lambda^i R_m^i \theta_m C_m^i + \lambda^{i-1} R_m^{i-1} \theta_m C_m^{i-1} & [\text{Decay and Production Terms}] \\
 & + \Sigma_m^i & [\text{Source Term}] \\
 & + X^i, & [\text{Matrix/Fracture Transfer Term}]
 \end{aligned} \tag{13-11}$$

where R is the retardation factor, θ is the moisture content, C is concentration (the unknown for which the equation is being solved), q is the groundwater flux, D is the dispersion coefficient, z is the elevation, λ is the radioactive-decay rate, Σ is the source term (zero everywhere except in the repository region), and X is the transfer term. The superscript i indicates a particular radionuclide and the subscript m indicates the matrix material. The equation for transport through the fractures is similar; a subscript f is simply substituted for the m subscript and the sign of the transfer term is reversed. The two coupled equations are solved for the concentration of each radionuclide at a given problem time. As indicated, the equations consist of terms describing the following phenomena: (1) movement of dissolved radionuclides in groundwater by advection and dispersion (including both molecular diffusion and hydrodynamic dispersion), (2) radioactive decay and production (when decay chains are specified) of radionuclides, (3) injection of radionuclides (when a source internal to the calculational mesh is specified—an external source is handled by a boundary condition), and (4) movement of radionuclides between the matrix and the fractures. The USATCONC source term model (see Chapter 11) is called by TOSPAC as a subroutine to provide the source term Σ .

The dispersion factor is a combination of molecular diffusion and hydrodynamic dispersion, and is defined separately in the matrix and the fractures as follows:

$$\begin{aligned}
 D_m^i &= \frac{D^i}{\tau_m} + \alpha_{Lm} |v_m|, & [\text{Matrix Diffusion and Dispersion}] \\
 D_f^i &= \frac{D^i}{\tau_f} + \alpha_{Lf} |v_f|, & [\text{Fracture Diffusion and Dispersion}]
 \end{aligned} \tag{13-12}$$

where D is the free diffusion coefficient in water, τ is the tortuosity-constrictivity factor, α_L is the longitudinal hydrodynamic dispersivity, and v is the pore-water velocity, or average linear velocity of the groundwater. Hydrodynamic dispersion occurs only downstream in the direction of flow; diffusion occurs both upstream and downstream; thus the dispersivities are taken to be zero above the repository.

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The retardation factor describes the geochemical effect of radionuclide sorption to the surface of the porous medium through which it is being transported. The retardation factors are given by

$$R_m^i = 1 + \frac{\rho_b K_d^i}{\theta_m}$$

$$R_f^i = 1$$

where ρ_b is the bulk density and K_d is the distribution coefficient. As indicated, no retardation on fracture walls was assumed.

The transfer term allows an approximation of the two-dimensional movement of solute between matrix and fracture "pores" in the one-dimensional TRANS. Two processes are included in the transfer term: advective transfer, in which radionuclides follow the movement of water between the matrix and fractures, and diffusive transfer, in which radionuclides follow the concentration gradient between the matrix and fractures. The equation for the transfer term is as follows:

$$\begin{aligned} X^i = & \left(\frac{\partial \theta_m}{\partial t} + \frac{\partial q_m}{\partial z} \right) C^i(b) && \text{[Advective Coupling]} \\ & + \gamma_d \frac{\theta_m D^i / \tau_m}{a^2} (C_f^i - C_m^i), && \text{[Diffusive Coupling]} \end{aligned} \quad (13-13)$$

where $C(b)$ is the concentration of a given radionuclide at the matrix/fracture boundary, a is one half of the distance between the centerlines of adjacent fractures (i.e., one half of the fracture spacing), and γ_d is the matrix/fracture coupling factor, an input variable that is used to set the strength of the interaction between the matrix and fractures. In this study, only one setting ($\gamma_d = 1$) was used for the matrix/fracture coupling. The value of $C(b)$ depends on whether water is flowing from matrix to fractures or vice-versa, and it is defined as follows:

$$C^i(b) = \begin{cases} C_f^i & \text{if } X_{advective}^i > 0; \\ C_m^i & \text{if } X_{advective}^i < 0. \end{cases} \quad (13-14)$$

13.3.2 Computational Model

The finite-difference method, which was used for the liquid flow calculations, was also used for the radionuclide transport calculations. An implicit differencing method was used for the time discretization (see Dudley et al., 1989, for details), so that time steps typically start out very small and grow to large values in order to be able to resolve the time-dependence of the solution at any given time.

Equation 13-11 and the corresponding equation for fracture concentration are solved for each radionuclide, leading to a system of $2N$ coupled equations, where N is the number of radionuclides being transported. The differencing scheme leads to a pentadiagonal matrix equation that can be solved very efficiently.

13.3.3 Applied Model

The same geometry and calculation mesh used in the flow calculations are used for the transport calculations (see Figure 13-7). Most of the parameters used by TRANS are presented in Chapter 5. As discussed there, 11 radionuclides were considered for aqueous transport (^{239}Pu , ^{237}Np , ^{238}U , ^{236}U , ^{235}U , ^{234}U , ^{233}U , ^{231}Pa , ^{129}I , ^{99}Tc , and ^{79}Se) and one for gaseous transport (^{14}C). For the Simple PA calculations, all 12 radionuclides were included in the TOSPAC transport calculation. The releases from the repository (calculated by USATCONC within TOSPAC) were saved and the ^{14}C releases used as input to GASTP for the gaseous-transport calculation. The amount of mass cross-

ing the bottom boundary each time step was also saved and those releases used as input to QEDTP for the saturated-zone aqueous-transport calculations. ^{14}C was included in both the TOSPAC and QEDTP transport calculations, but its releases were not used in calculating the final CCDF. The gaseous ^{14}C releases were used instead.

Initial and boundary conditions are required for the transport calculation. The initial condition used is zero concentration everywhere. The top boundary condition is zero concentration flux and the bottom boundary condition is zero concentration for all radionuclides, and separately for matrix and fracture concentrations.

13.3.4 Transport Results

Some examples of unsaturated-zone transport results are shown in Figures 13-14 through 13-16. These results were obtained using median values for all input parameters, and are for the mixed-waste case with horizontal emplacement.

Figure 13-14 shows ^{99}Tc concentration in the unsaturated zone for several times within the 10,000-yr calculation period. As seen in the figure, very little ^{99}Tc reaches the water table within 10,000 yr. However, ^{99}Tc is very mobile compared to most of the radionuclides; Figure 13-15 shows ^{237}Np concentration, and it can be seen that ^{237}Np moves only about 30 m in 10,000 yr, compared to about 200 m for ^{99}Tc .

Figure 13-16 shows cumulative radioactivity reaching the water table as a function of time. Only ^{99}Tc and ^{129}I are shown, because all of the other radionuclides are off the scale (i.e., less than 10^{-12} Ci in 10,000 yr). The releases shown in Figure 13-16 are far down on the breakthrough curve, as can be seen from Figure 13-14. Thus, they depend sensitively on the assumptions made about hydrodynamic dispersion; if there were no hydrodynamic dispersion, there would be no releases to the water table within 10,000 yr.

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Figure 13-14. Concentration for ^{99}Tc in the unsaturated zone for six times within the 10,000-yr regulatory period.

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Figure 13-15. Concentration for ^{237}Np in the unsaturated zone for six times within the 10,000-yr regulatory period.

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Figure 13-16. Cumulative radioactivity reaching the water table as a function of time.

13.4 Gaseous Carbon-14 Transport

Results from the TGIF gas flow model (Section 13.2.5) were used to construct a simple mathematical model (GASTP) of the cumulative release of ^{14}C to the accessible environment. A complete derivation and discussion of the formula behind this model has not appeared in earlier reports (but see Sections 3.1.2 - 3.1.3 of Lin et al., 1986, where a similar formula is derived and applied to liquid-phase transport in the vadose zone of the Yucca Mountain Repository Site), so one is provided below.

13.4.1 Derivation of the GASTP Equation

The equation describing transport of $^{14}\text{CO}_2$ in a steady, incompressible gas flow through the overburden of a vadose-zone repository is

$$\frac{\partial c}{\partial t} + \frac{\bar{u}}{r\theta} \cdot \nabla c = -\lambda c \quad (13-15)$$

where:

- $c(\bar{x}, t)$ is concentration of ^{14}C in $\text{kg}/(\text{m}^3\text{-air})$ at position $\bar{x}$ and time $t > 0$;
- $\theta(\bar{x})$ is porosity of the medium (dimensionless) at position $\bar{x}$;
- $r(\bar{x})$ is a retardation factor (dimensionless) owing to the time ^{14}C spends in the relatively immobile liquid phase as dissolved bicarbonate;
- $\bar{u}(\bar{x})$ is specific discharge of air [$\text{m}^3\text{-air}/(\text{m}^2\text{-bulk solid}) \cdot \text{s}$]; note that in steady, incompressible flow, $\nabla \cdot \bar{u} = 0$;
- λ is decay rate of ^{14}C ($1.2097 \times 10^{-4} \text{ s}^{-1}$).

In view of the condition $\nabla \cdot \bar{u} = 0$, gas flow can be viewed as taking place along stationary tubes of flux that connect the repository with the atmosphere; a typical flux tube is sketched in Figure 13-17. Let ℓ be distance along a flux tube measured positive in the direction of flow, with $\ell = 0$ at the point where the flow line exits the repository. Then it follows that $d\ell/dt = |\bar{u}|$ and

$$\frac{\partial c}{\partial \ell} = \frac{1}{|\bar{u}|} \bar{u} \cdot \nabla c$$

Equation 13-13 may then be written as

$$\frac{\partial c}{\partial t} + \frac{|\bar{u}|}{r\theta} \frac{\partial c}{\partial \ell} = -\lambda c \quad (13-16)$$

Equation 13-14 can be further simplified by introducing the notion of *transport time* along a flow tube:

$$T(\ell) = \int_0^\ell \frac{r\theta}{|\bar{u}|} d\ell \quad (13-17)$$

and noting that

$$\frac{\partial c}{\partial T} = \frac{\partial c}{\partial \ell} \frac{d\ell}{dT} = \frac{|\bar{u}|}{r\theta} \frac{\partial c}{\partial \ell}.$$

It follows that Equation 13-16 can be written in its simplest form as

$$\frac{\partial c}{\partial t} + \frac{\partial c}{\partial T} = -\lambda c, \quad T > 0, t > 0. \quad (13-18)$$

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Figure 13-17. A stationary tube of flux that connects repository with the atmosphere. Discharge (flux times area) is constant at any point $\ell \geq 0$ along streamline.

This equation is to be solved subject to the initial condition,

$$c(T, 0) = 0, \quad T > 0, \quad (13-19)$$

and the boundary condition,

$$c(0, t) = \frac{q(t)}{D}, \quad t \geq 0. \quad (13-20)$$

where $q(t)$ is the rate at which ^{14}C is released in the repository (kg/s) owing to failures of waste containers, and

$$D = \iint_{AR} \vec{u} \cdot \vec{n} \, dA \quad (13-21)$$

is the net discharge of air through the repository ($\text{m}^3\text{-air/s}$), a quantity independent of time in steady-state flow. In Equation 13-21, AR is the effective area of the walls of those repository regions that contain waste; $\vec{n}$ is a local unit vector pointing outward from the walls, and dA is an element of area.

Note that boundary condition Equation 13-20 is only an approximation to the concentration of ^{14}C in the air-filled void spaces of the repository at any time; its form follows from assumptions that the mean residence time of air in the repository is small in comparison with the ^{14}C half life and typical travel times to the atmosphere. As will be seen, these and one more assumption permit the construction of a model that does not require knowledge of D , the net discharge of air through the repository.

Equations 13-18 to 13-20 can be solved by a variety of methods (e.g., the Laplace Transform). The solution is

$$c(T, t) = \frac{e^{-\lambda T}}{D} q(t - T)h(t - T) \quad (13-22)$$

where $h(x)$ is the unit step function defined by $h(x) = 1$ if $x \geq 0$, and $h(x) = 0$ otherwise. This equation gives the concentration of ^{14}C (in $\text{kg/m}^3\text{-air}$) at time $t > 0$ and at any point $\ell > 0$ along a flux tube that corresponds to a transport time $T(\ell)$. Without loss of generality, we can now eliminate any reference to distance along a flux tube and interpret T simply as transport time to a point on the surface defining the overburden-atmosphere interface. Define

$$f(T)dT = \text{the fraction of flow tubes that have transport times to the atmosphere between } T \text{ and } T + dT. \quad (13-23)$$

with the understanding that some flow tubes may have very long transport times to the atmosphere, so that

$$\int_0^{\infty} f(T)dT = 1.$$

The quantity $f(T)$ is obviously identical to the *probability density function* for transport time, i.e., the probability that any molecule of $^{14}\text{CO}_2$ released from the repository at time zero will arrive at the soil-atmosphere boundary in a time interval T to $T + dT$. In a steady flow field, the differential air discharge to the atmosphere from paths with transport times between T and $T + dT$ may then be represented as

$$d\Phi(T) = Df(T)dT \quad \text{m}^3 - \text{air/s}$$

and so the total rate of release of ^{14}C to the atmosphere at time $t > 0$ is

$$\dot{m}_A(t) = \int_0^{\infty} c(T, t) d\Phi(T) = \int_0^t e^{-\lambda T} q(t-T) f(T) dT \quad \text{kg/s} \quad (13-24)$$

where the last expression in Equation 13-24 is obtained by substitution of the expression for $c(T, t)$ from Equation 13-22. Note that reference to D , the net discharge of air through the repository, has been eliminated.

The cumulative mass of ^{14}C released to the atmosphere by time $t > 0$ is the integral over time of the mass release rate:

$$M_A(t) = \int_0^t \dot{m}_A(t') dt' \quad (13-25)$$

Equations 13-24 and 13-25 are the basic equations of the GASTP model. Given the functions $q(t)$ and $f(T)$, the integrations indicated in these equations are performed numerically, first to obtain the mass release rate function, $\dot{m}_A(t)$, and then to compute the cumulative mass released to the atmosphere, $M_A(t)$. Limitations of this model are discussed below, but first the source of the transport time distributions, $f(T)$, appearing in Equation 13-24 is described.

13.4.2 Transport Time Distributions

Ross and coworkers (Ross et al., 1992) have used the TGIF gas flow model (13.1.14) and particle-tracking techniques to construct empirical transport time distributions for four values of constant repository temperature, 300, 315, 330, and 360 K (Figure 13-18; empirical distributions are irregular curves). In computing a particle's motion through the repository overburden, steady velocity fields similar to the one shown in Figure 13-13 for 330 K were used (note that "velocity" here means specific discharge over porosity, i.e., $\bar{u}/\theta$). In addition to repository temperature, the velocity fields also depend strongly upon permeabilities assigned to the welded and non-welded tuff units of the overburden. The empirical transport time distributions in Figure 13-18 were based on a 10^{-11} m^2 permeability for welded units and a 10^{-13} m^2 permeability for nonwelded units. In addition, all velocity fields were converted to effective transport velocities for $^{14}\text{CO}_2$ by dividing by a temperature-dependent retardation factor r (Figure 13-19).

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Figure 13-18. Empirical and fitted distributions of transport time for ¹⁴CO₂ through overburden of Yucca Mountain repository site (see text). Irregular curves are empirical CDFs; smooth curves are lognormal fits to empirical CDFs.

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Figure 13-19. Retardation factor as a function of temperature for all units (taken from Figure 4-2 of Ross et al., 1992).

To keep the GASTP model numerically simple, the empirical transport time distributions supplied in Ross et al., 1992 were fitted with lognormal distributions which have probability density functions of the form

$$f(t) = \frac{1}{\sqrt{2\pi\xi t}} \exp \left[-\frac{(\ln t - \mu)^2}{2\xi^2} \right] \quad (13-26)$$

The sample means and standard deviations of the empirical distributions shown in Figure 13-18 (here denoted by $\bar{T}$, σ_s) were calculated and used to determine the parameters μ and ξ in Equation 13-26 as functions of temperature (Table 13-2). The cumulative lognormal distributions obtained by this procedure are the smooth curves that roughly coincide with the empirical distributions in Figure 13-18.

The fit between empirical and analytic distributions could be improved considerably by fitting each empirical curve to a convex combination of lognormals (note the clear bimodality of some of the empirical CDFs).

Table 13-2. Sample Means, Standard Deviations, and Fitted Lognormal Parameters for Transport Time Distributions as Functions of Temperature.

Temperature (K)	$\bar{T}(y)$	$\sigma_s(y)$	$\mu[\ln(y)]$	$\xi[\ln(y)]$
300	21440.6	6313.1	9.9315	0.28835
315	8155.0	3881.6	8.9043	0.45194
330	4287.4	3855.5	8.0671	0.76981
360	1516.5	838.3	7.1908	0.51639

13.5 Radionuclide Transport in Saturated Zone

Lateral transport in the saturated zone was calculated for the Simple PA with a dual-porosity modeling code, QEDTP. QEDTP is a modified version of the analytical two-dimensional model used in the scoping calculations for the 1993 PA (Rechard, Ed., 1993, Appendix C). The code was modified to account for the flux through the boundary $x_1 = X_B$ due to dispersion; although the effect of this term represents only a few percent of the total flux, it is included here for completeness.

The following simplifications were assumed for calculating radionuclide releases due to groundwater transport:

- The flow field is assumed to be constant over the 10,000-yr regulatory period. Under the assumption of uniform flow, the flow field is completely characterized by pathline distance and travel time, which were derived from the TSPA-1993 performance assessment for the Yucca Mountain Project. Travel distance and time were assumed to be independent.
- Radionuclides move as passive tracers and do not chemically interact with the matrix or fracture filling material, i.e., the distribution coefficients, K_D , are zero. A future version of QEDTP will remove this constraint.
- The release due to transport through spatially variable flow fields is approximated by the release due to transport through a uniform flow field representing a stream tube around the actual (tortuous) pathway.

Dagan (1982), citing Carslaw and Jaeger (1959), presents a solution for concentration due to introduction into a uniform flow field of a mass Δm at the origin at time 0:

$$\Delta c_s(\mathbf{x}, t) = \frac{\Delta m}{n} \frac{1}{4\pi(D_I D_{II})^{1/2} t} \exp \left[-\left\{ \frac{(x_1 - Ut)^2}{4D_I t} + \frac{x_2^2}{4D_{II} t} \right\} \right] \quad (13-27)$$

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where:

Δc_s	=	concentration (mass/volume) of a stable isotope,
$\mathbf{x}=(x_1, x_2)$	=	position,
t	=	time since introduction of Δm ,
n	=	medium porosity,
D_x	=	dispersion coefficients,
U	=	fluid velocity.

Coordinate x_1 is assumed to be aligned along the flow direction. If the tracer undergoes radioactive decay, and the daughter products are transported in the same way as the parent, then the concentrations of daughter products at any point are given by the solution of the Bateman equations:

$$\Delta c_i(\mathbf{x}, t) = \lambda_1 \lambda_2 \dots \lambda_{i-1} \Delta c_s(\mathbf{x}, t) \sum_{j=1}^i \frac{e^{-\lambda_j t}}{\prod_{k \neq j} (\lambda_k - \lambda_j)} \quad (13-28)$$

The unsaturated zone discharge from TOSPAC, which forms the source-term for the lateral transport model, is given as a series of $\Delta m(t)$ per time step. The total mass released through the lateral discharge boundary during an interval can be calculated in the following way:

- The mass introduced over each interval is assumed to be introduced in a pulse at the center of the interval.
- Equations 13-27 and 13-28 are used to derive the integrated release associated with the interval mass.
- The total integrated release is the sum of the release for all source intervals.

This method relies (among other things) on the assumption that the interval size is small relative to the half-life of the tracer, and that the travel time is large relative to interval size. These assumptions seem reasonable given the time step typically used in TOSPAC, but have not yet been properly evaluated. Other methods of release calculation can be predicated on Equation 13-28 if either of these conditions does not hold.

Assuming that the dispersive flux is negligible for the purpose of calculating integrated release, the mass flux density of radionuclide i is:

$$\Delta q_i(\mathbf{x}, t) = nU \Delta c_i(\mathbf{x}, t) \quad (13-29)$$

While the integrated discharge rate across an infinite boundary perpendicular to flow at $x_1 = X_B$ is given by:

$$\begin{aligned} \Delta Q_i(t) &= \int_{-\infty}^{\infty} \Delta q_i(\mathbf{x}, t) dx_2 \Big|_{x_1=X_B} = nU \int_{-\infty}^{\infty} \Delta c_i(\mathbf{x}, t) dx_2 \Big|_{x_1=X_B} \\ &= \lambda_1 \lambda_2 \dots \lambda_{i-1} \Delta Q_s(\mathbf{x}, t) \sum_{j=1}^i \frac{e^{-\lambda_j t}}{\prod_{k \neq j} (\lambda_k - \lambda_j)} \end{aligned} \quad (13-30)$$

where,

$$\Delta Q_s(t) = \int_{-\infty}^{\infty} \Delta c_s(\mathbf{x}, t) dx_2 \Big|_{x_1=X_B} = \frac{\Delta m U}{2(\pi D_I t)^{1/2}} \exp \left[-\frac{(X_B - Ut)^2}{4 D_I t} \right]$$

The total amount of each radionuclide released due to Δm is given by:

$$\Delta R_i(t) = \int_0^t \Delta Q_i(\tau) d\tau$$

Taking note of the time dependencies in Equation 13-30, $\Delta R_i(t)$ is evidently a linear combination of the form,

$$\Delta R_i(t) = \lambda_1 \lambda_2 \dots \lambda_{i-1} \sum_{j=1}^i \frac{\Delta D(\lambda_j, t)}{\prod_{k \neq j} (\lambda_k - \lambda_j)}$$

where,

$$\begin{aligned} \Delta D(\lambda, t) &= \int_0^t e^{-\lambda \tau} \Delta Q_s(\tau) d\tau \\ &= \frac{\Delta m U}{2} d\tau \int_0^t \frac{e^{-\lambda \tau}}{(\pi D_I \tau)^{1/2}} \exp \left[-\frac{(X_B - U\tau)^2}{4 D_I \tau} \right] \\ &= \frac{\Delta m}{2\beta} \left(e^{\frac{X_D}{2}(1-\beta)} \operatorname{erfc} \left[\frac{1}{2} \sqrt{X_D X_A} \left(1 - \frac{\beta}{X_A} \right) \right] \right. \\ &\quad \left. - \left(e^{\frac{X_D}{2}(1+\beta)} \operatorname{erfc} \left[\frac{1}{2} \sqrt{X_D X_A} \left(1 + \frac{\beta}{X_A} \right) \right] \right) \right] \end{aligned} \quad (13-31)$$

where,

$$\begin{aligned} X_D &= \frac{X_B}{\alpha_I} \\ X_A &= \frac{X_B}{U t} \\ \beta &= \sqrt{1 + 4 \frac{\lambda \alpha_I}{U}} \end{aligned}$$

To account for the flux due to dispersion, that is the term $\Delta q_i(\mathbf{x}, t) = n D_I \frac{\partial}{\partial x} \Delta c_i(\mathbf{x}, t) \Big|_{x_1=X_B}$, Equation 13-31 becomes

$$\begin{aligned} \Delta D(\lambda, t) &= \frac{\Delta m}{4} \left\{ \left(1 + \frac{1}{\beta} \right) e^{\frac{X_D}{2}(1-\beta)} \operatorname{erfc} \left[\frac{1}{2} \sqrt{X_D X_A} \left(1 - \frac{\beta}{X_A} \right) \right] + \right. \\ &\quad \left. \left(1 - \frac{1}{\beta} \right) e^{\frac{X_D}{2}(1+\beta)} \operatorname{erfc} \left[\frac{1}{2} \sqrt{X_D X_A} \left(1 + \frac{\beta}{X_A} \right) \right] \right\} \end{aligned} \quad (13-32)$$

Equation 13-32 was used in the calculations.

14. Biosphere Modeling

R. D. McCurley and L. J. Rahal

14.1 Introduction

In anticipation of evolving changes in regulatory requirements for repositories, dose calculations were performed for the 1994 PA. A supplementary code, GENII-S, was used that accepts performance assessment release estimates as input data, adds exposure-route, human-dose, and human-dosimetry modules, and combines their results to produce estimates of the internationally accepted indices by which human health effects are assessed (Napier et al., 1988a,b,c; Leigh et al., 1993). In the present analysis, guidance provided by the International Commission on Radiological Protection (ICRP, 1985), the National Council on Radiation Protection and Measurements (1984), and the Nuclear Energy Agency (NEA, 1984) was followed. Present surface climatological conditions and demographics were assumed to persist for 10,000 years or to peak arrival times. The "maximum individual" was assumed to live and work at the precise location and time that would lead to the highest possible doses. For waterborne exposure scenarios, doses and health effects are reported for the maximum individual.

For the dose calculations in the 1994 PA, three disposal systems were considered: salt, granite, and tuff. Calculations were run for the salt and granite sites so that results between conditions examined in the 1993 and 1994 PAs could be compared. However, because differences exist between the two performance assessments in inventory and analysis techniques, conclusions about the relative effectiveness of different repositories must be regarded cautiously.

14.1.1 Exposure Scenarios for Determining Dose to Humans

Exposure scenarios for the 1994 PA are based on inadvertent human intrusion, which consists of drilling into the repository or of accessing contaminated groundwater downgradient from the repository at some time after loss of institutional control, which occurs after 100 yr of closure.

For these performance calculations, exposure scenarios on the surface begin either at the head of a well with a sludge pond containing cuttings/cavings (material eroded from the borehole wall), at a farm site downwind of the well, at a nearby well through which contaminated groundwater is pumped to the surface, or at a freshwater lake partially fed by a contaminated aquifer. The hypothetical well and lake are assumed to be located downgradient from the waste. These exposure pathways are illustrated in Figures 14-1a through 14-1c.

14.1.2 Methodology as it Relates to 40 CFR 191 and RCRA Regulations

All calculations for the 1994 PA are performed with a view toward eventual comparison with 40 CFR 191. They therefore tend to employ complementary cumulative distribution functions (CCDFs) to assess sensitivities of the modeling system to specific conceptual model uncertainties (Helton et al., 1992). It is tempting to use these CCDFs to test compliance. However, because the models are preliminary, the CCDFs are also preliminary and are therefore not wholly suitable for final compliance evaluations with 40 CFR 191.

14.2 Description of Critical Pathways

Pathway groups, which are collections of exposure pathways to humans, are considered for the tuff, salt, and granite disposal systems. The pathways differ per geologic medium based on the characteristics of the individual site. Also, different source terms were considered, depending on the site. For the salt and granite disposal systems, source terms from Waste Disposal Group 1 as defined in the 1993 PA were used for exposure scenarios that use data from cuttings/cavings results (e.g., driller scenario). For the tuff disposal system, cuttings and transport data for the combined waste group as modeled in the Complex PA are used.

14. Biosphere Modeling

Figure 14-1. Exposure pathways used in the 1994 PA for (a) special geometries, (i.e., cuttings, external only) (b) groundwater transport, and (c) atmospheric transport.

The five main pathway groups are as follows: (a) Driller Exposure Pathway (Case 1); (b) Farm Pathway (Case 2a) and Farm Stockpond Pathway (Case 2b); (c) Rancher Pathway (Case 3); (d) Lake Exposure Pathway (Case 4), and (e) Farm Well Pathway (Case 5). The pathways for each disposal system are described below.

The term "pathway group" refers to a sequence of hypothetical pathways by which radionuclides from a repository reach humans. The sequence may consist of only one pathway, as in Case 3, where only ingested meat is considered. Alternatively, there may be several simultaneous pathways (e.g., ingestion, inhalation, external exposure), as in Case 2 for the farm family. All pathway groups for the salt repository assume that an inadvertent borehole intrusion into the repository occurs at some time after loss of institutional control. As stated in the executive summary (Volume 1), the permeability of the fractures in the granite and tuff was assumed to be high enough that additional fluid paths created by the drilled boreholes would not significantly enhance fluid movement and radionuclide transport. The first pathway group, Case 1, actually coincides with the inadvertent intrusion event and thus it is considered for all sites.

In the discussion that follows, each pathway group is described separately since the nature and mechanism of contaminant transport vary from group to group. Also note that for the Case 2a, Case 2b, and Case 3 pathways, ^{210}Pb is not transported through the aquifer. However, this radionuclide still plays an important role in terms of consequent doses to humans and it therefore appears in the GENII-S result. ^{210}Pb is assumed to be in secular equilibrium with ^{226}Ra , which is long-lived relative to ^{210}Pb . The radionuclides that are transported through the aquifer from the borehole, along with their groundwater concentrations at the point of extraction for the stockpond, are listed in Section 14.4. The radionuclide concentrations of exhumed material resulting from drilling activities are also listed in Section 14.4.

14.2.1 Driller Exposure Pathway

For the Driller Exposure Pathway (Case 1), the data retrieved from the cuttings calculation database represented the total curies per radionuclide found in a hypothetical sludge pit. For the salt and granite repositories, the 1993 inventory characterization considered several waste groups, each consisting of several distinct waste parcels (see Rechard, Ed., 1993). The waste group considered here is referenced as Waste Disposal Group 1 and includes parcels indicated in the 1993 report (see Rechard, Ed., 1993, Chapter 4). For the tuff repository, see description in Section 14.3.1. The driller exposure doses depend both on examination of a sample contaminated rock assumed to have the same concentration of radioisotope contamination as characterized by repository-depth drill material and exposure to groundshine created by the cuttings in the nearby sludge pit, the area of which is about 100 m^2 . Inhalation is not considered as a pathway because the material remains as a fluid mixture. The size of the sludge pit depends primarily on the size of the hypothetical intrusion borehole. The expression used to determine the dimensions of the sludge pit was given in a memo from Tom Blaine (personal communication) as follows:

$$\text{Width (m)} = \{ \text{Volume (drill hole)}(\text{m}^3) * \# \text{gal/m}^3 * 2.0 / (2.125 * 7.5)(\text{ft-gal}^{-1}) \} * 0.3048 (\text{m/ft}), \quad (14.2-1)$$

where the width is in meters and the volume of the borehole is in cubic meters.

$$\text{Length} = 2.5 * \text{Width}$$

$$\text{Depth} = 0.85 * \text{Width}$$

The borehole radius used in the calculations for the salt and granite sites was 0.3048 m, the median value listed in Volume 1 of Rechard, Ed., 1993. The borehole radius is a sampled parameter for the tuff site. The length of the borehole is assumed equivalent to the depth of the repository below the surface (longer boreholes would make the calculations less conservative).

Assuming that a typical chip would have the same concentrations (on average) as the material in the sludge pit, and knowing the average density of the dry volume of the sludge material, the chip concentrations, $C(\text{Ci/m}^3)$ are given by:

$$C(\text{chip}) = C(\text{pit}) / [0.5 * \text{density (soil)} * \text{volume (pit)}] \quad (14.2-2)$$

where the 0.5 represents the fact that half the pit volume is water. The density is the average density of the excavated material and C is the total removed curies for nuclide k found in the pit. The chip was assumed to be spherical with the radius of 0.05 m. The chip has a density equal to the average density of exhumed rock, chosen to be 1400 kg/m³. The spherical geometry was assumed for mathematical symmetry in calculating external dose conversion factors.

14.2.2 Farm and Farm Stockpond Pathways (Cases 2a and 2b)

Farm Pathway (Case 2a). The Farm Pathway group involves two temporarily and spatially distinct sources of contamination, namely: (a) a dried and wind-scoured sludge pit (Case 2a, Farm Pathway), and/or (b) a dried-up stockpond (Case 2b, Farm Stockpond Pathway). The overall temporal sequence of the entire suite of "pathway" events would be the following: (i) Case 1 pathway of driller exposure at the time of intrusion, (ii) the Case 2a pathway where the contamination source is a dried-up sludge pit, (iii) the Case 3 pathway (see Section 14.2.3), and finally, (iv) the Case 2b pathway where the source of contamination is a dried-up stock pond. The groundwater flow models used to provide data for these calculations (and for the water source scenarios considered for the other repositories) treat two-phase flow and dual porosity (see Chapters 12 and 13).

For this pathway (Case 2a), the data retrieved from the cuttings calculations represent the total curies per radionuclide of cuttings deposited into a hypothetical sludge pit resulting from an exploratory hydrocarbon drilling operation. The sludge pit is assumed to dry out completely so that contaminated soils can be air suspended and transported downwind onto a hypothetical farm. The thickness of the soil available for resuspension in the sludge pit is assumed to be 1.0 cm (U.S. DOE, 1980, Section K.3.1, p. K-26). The thickness of soil available for resuspension at the farm site is assumed to be 15 cm. The period over which the wind deposits contaminated dust onto the farm is assumed to be 100 yr. This period was chosen because a steady state between two competing processes, deposition and infiltration through the bottom of the arable soil, is obtained in about that time period. Knowing the pit dimensions, and especially the depth of the pit, the total number of curies suspended in the air per year can be calculated. An expression from US DOE (1980) was used; the flux rate, Q (kg/s), being given by

$$Q = K_r \rho_s A_s \Delta x_s \hat{U}_w^3 \quad (14.2-3)$$

where

- K_r = resuspension constant (s²/m³),
- ρ_s = density of surface soil available for resuspension (kg/m³),
- A_s = surface area of soil available for resuspension (m²),
- Δx_s = depth of soil available for resuspension (m),
- $\hat{U}_w$ = mean wind speed (m/s).

The resuspension factor K was taken to be 1.0×10^{-13} where U is the average wind speed in m/s. The factor (1.0×10^{-13}) is applicable in semi-arid environments. The average wind speed used was 3.7 m/s; the soil density is assumed to be 1.4×10^{-3} kg/m³. The area of the sludge pit is given above.

The farm is assumed to be located 2400 km downwind from the sludge pit, beyond the land-withdrawal boundary. Because the area of the sludge pit is 100 m², it can be considered a point source as far as the farm is concerned. Using a squared Gaussian plume model (U.S. DOE, 1980, see Section K.3.1, p. K-25) excerpted from that report, the ratio of ground-level concentrations at the farm (Ci/m³) to the source strength, χ/Q , can be calculated as:

$$\chi/Q = 2.0 / [3.0 * (2.0 * \pi)^{1/2} * \sigma_y \sigma_z * U], \quad (14.2-4)$$

where

- σ_y = $0.11 * D * (1.0 + 10^{-4} * D)^{-1/2}$ (dispersion coefficient),
- σ_z = $0.08 * D * (1.0 + 2.0 * 10^{-4} * D)^{-1/2}$ (dispersion coefficient),
- D = downwind transport distance,
- U = average wind speed.

NOTE: The expressions for σ_y , σ_z , given above, represent slightly unstable lower atmospheric conditions typical of the desert in the southwestern United States and are considered appropriate for this analysis.

Farm Stockpond Pathway (Case 2b). The conditions for the Farm Stockpond Pathway are similar to the Farm Pathway. Differences between the pathways are noted below.

The air concentrations are determined in the same manner as described for the Farm Pathway, except the soil concentrations result from a gradual drying up of the stockpond that originally supplied the cattle (see Rancher Pathway, below). It was assumed that all the radiological contamination in the water became mixed with the top 1 cm of soil in the dried pond, which was then resuspended by the wind as described previously and redeposited on the surface at a neighboring farm.

In this case, however, the farm is located only 500 m from the dried pond. Thus, the χ/Q ratio described previously is somewhat larger than in the Farm Pathway. However, both the inventory and concentrations in the dried stockpond are much smaller than those in dried sludge pits. Consequently, this stockpond source turned out to be a less significant pathway group than the previous farm family scenario.

14.2.3 Rancher Pathway

This pathway (Case 3) involves exposure to persons living on a cattle ranch, who consume meat from their cattle. The cattle drink water from a contaminated stockpond. Meat is assumed to be the only food consumed. No other pathways are considered.

An examination of 1993 PA contour plots of plume concentrations at the 2.4-km (land-withdrawal) boundary "downstream" from the hypothetical intrusion borehole suggested locations thought to be representative of maximal concentrations (in space). The orientation of the groundwater concentration plumes with respect to the modeled transport domain suggests the 2.4-km boundary may be modeled simply as a connected collinear set of nodes parallel to the horizontal axis. An examination of similar plots from randomly selected vectors showed this conjecture to be generally true. Three locations, spaced equidistantly within this bounded region on the southern boundary, were selected as representative of maximal concentrations for the 20 vectors for each waste group considered. These three locations correspond to nodes in the mesh of the local domain used by STAFF2D in the 1993 PA, nodes where a hypothetical test-case stockwell might be located. Finally, from an examination of the output from these three candidate locations, one location was selected as the maximal set for input to GENII-S. (Concentrations in the groundwater at this spatial location have not peaked at the time selected, about 10,000 yr from closure.)

Once a critical site (or sites) for a typical stockpond was selected, it was necessary to determine how much water must be pumped (from the aquifer) to satisfy drinking requirements of typical cattle in the area. Cows living in and about the area drink, typically, about 10 m^3 of water per year. Assuming (i) a stockwell can supply the water needs for 25 cattle, and (ii) the local evaporation rate is about $25 \text{ m}^3/\text{yr}$, roughly $275 \text{ m}^3/\text{yr}$ of water must be pumped annually. Typically, pumping occurs during seven months of the year, or about 60% of the time. Thus, to provide the required water, a typical pumping rate must be about $4.67 \times 10^{-7} \text{ m}^3/\text{s}$ (T. Blaine, personal communication).

The local grid in which transport calculations were carried out is described in Chapters 12 and 13 of Rechar, Ed. (1993). It is assumed that the influence of the stockwell would extend to a locus defined by a cell of this mesh centered at that node where the stockwell intrusion is located. Because the elements are squares 125 m on a side, this point amounts to considering a radius of influence of 62.5 m. This value appears to be a very safe assumption because the effects on the subsurface movement of brine from the presence of the pumping well are very small at a 50-m radius. Sustaining a steady-state flow at the well, assuming an aquifer thickness of about 1 m, requires a flow rate of about $4 \times 10^{-9} \text{ m}^3/\text{s}$, which is considerably less than the typical flow rates found in the aquifer at the chosen locations. Thus, the concentrations and flow rates at the chosen nodal locations are reasonable for determining the amount of water available for pumping and the extent of radiological contamination in that water. Additionally, the water consumed by the cattle should not have a brine concentration greater than seven parts per thousand or a specific gravity greater than 1.007. Because many of the vectors showed concentrations greater than that limit, another hypo-

thetical source of fresh water was supplied to dilute the brine concentrations adequately (i.e., so the resultant brine concentration was at the maximum allowed value).

14.2.4 Lake Exposure Pathway

The Lake Exposure Pathway (Case 4) is another plausible source of significant dose to humans. Here, we consider a family who lives near a lake and whose subsistence depends significantly on the lake water, which has been contaminated by a groundwater source. Exposure occurs from the following sources: (1) human drinking water, (2) farm animals drinking water and human ingestion of milk, eggs, and meat from the farm animals, (3) irrigation water and subsequent ingestion of fruits and vegetables grown in the family garden, (4) aquatic foods from the lake, i.e., fish, (5) recreational exposure, and (6) external exposure to water while fishing.

The lake is assumed to be fed by a single groundwater well that is contaminated. The flux rate is determined by flow rates from the transport calculations. The concentration of the contaminated water entering the lake is assumed to be the same as that near and downstream from a secondary fracture connecting the repository to the lower aquifer, where most flow from the repository occurs. The lake is also fed by net precipitation resulting from two factors: (1) rainfall/snowfall and (2) evapotranspiration. Also, the catchment area size, if larger than the lake area, causes additional precipitation to flow into the lake. The lake area ($5.129 \times 10^6 \text{ m}^2$), depth (4.365 m), and the net precipitation (0.344 m/yr) are from Mehta (1985).

14.2.5 Farm Well Pathway

The Farm Well Pathway (Case 5) represents a source of significant dose to humans through the use of groundwater for farming activities and for drinking. A hypothetical water well withdraws contaminated water from the lower fracture zone passing beneath the repository. Concentrations in the well water are the same as concentrations at the intersection of the well with the lower aquifer. It is assumed that enough water is supplied by the aquifer to support modest farm activities (drinking water and irrigation). A well is located so that it finds water of maximal contamination at selected distances from the repository. Individuals on the farm are exposed by drinking contaminated well water, eating crops irrigated by contaminated water, and using products from animals that drink contaminated water and eat grains grown on the farm.

14.3 Pathway Descriptions by Repository

14.3.1 Tuff Repository

The exposure pathways that were modeled for the tuff site are (a) driller exposure pathway (Case 1) and (b) farm well pathway (Case 5) that includes a well for drinking water and irrigation at several locations at the repository horizon. The well extracts contaminated water from the aquifer. For the tuff site, dose calculations for the 1994 PA used inventories for the mixed waste group modeled in the Complex PA and considered both vertical and horizontal emplacement.

The Driller Exposure Pathway (Case 1) for the tuff repository is similar to the pathway described in Section 14.2.1 with the following exceptions. First, the drill bit diameter was sampled using a delta distribution with 36 samples (vectors). Again, both vertical and horizontal emplacement are considered; additionally, for the horizontal emplacement, calculations of dose were performed assuming (a) the entire waste parcel was removed and (b) the volume given by two drill bit diameters was removed. However, only 16 distinct drill bit diameters were used (see Chapter 8 for more details). Second, for the dose calculations, the pit dimensions depend inversely on the drill bit diameter (amount of material exhumed). The concentration (Ci/kg), and thus the dose, vary inversely with the square

of the drill bit diameter (or the volume of material exhumed), so there is a resulting distribution of dose. The drill depth for the tuff repository was assumed to be 300 m.

The Farm Well Pathway (Case 5) for the tuff repository is similar to the pathway described in Section 14.2.5. A hypothetical farm is located at the surface location marking the edge of the repository and at distances of 500, 1000, 2400, and 5000 meters from this location and accesses a contaminated source of groundwater from the aquifer by means of well extraction. The concentrations in the groundwater are those corresponding to a period 10,000 yr after closure. Examination of groundwater concentrations at 2400 m and 5000 m showed that doses would be negligible. These locations represent a worst-case scenario in terms of accessing contaminated groundwater, given the variation of contaminant plume over the selected realizations. A well drilled into the aquifer could supply enough water to support a small farm without disturbing the flow field utilized in the saturated transport calculations. (Eslinger et al., 1993, estimated the value at 1.8×10^7 l/yr.) The farm family raises enough stock, poultry, vegetables, and fruits for its own needs. The Rancher Pathway is not considered separately because it is a subgroup of the Farm Well Pathway. No farm family scenarios using resuspension of dried particulates are considered here, but might be in future studies.

14.3.2 Salt Repository

The four main exposure pathway groups considered for the salt repository are

- Driller Exposure Pathway (Case 1)
- Farm Pathway (Case 2a)
- Farm Stockpond Pathway (Case 2b)
- Rancher Pathway (Case 3)

These pathways are described in Sections 14.2.1, 14.2.2, and 14.2.3, respectively. As described in Rechar, Ed. (1993), Waste Disposal Group 1 for the salt repository includes Waste Parcels 1, and 4 through 9. The drill depth for the salt repository is assumed to be 700 m. Concentrations in the groundwater occur at approximately 10,000 yr after closure (i.e., 9000 yr after an intrusion by drilling into the repository, which occurred at 1000 yr).

14.3.3 Granite Repository

The three exposure pathways for the granite repository include driller exploration of hydrocarbons (Driller Exposure Pathway, Case 1), the Lake Exposure Pathway (Case 4) and the Farm Well Pathway (Case 5) as described in Sections 14.2.1, 14.2.4, and 14.2.5, respectively.

The Rancher Pathway (Case 3) is not considered for the granite site. The Lake Exposure Pathway (Case 4) actually includes the Rancher Pathway as a subgroup, with the lake serving as a stockpond. Exposure from resuspension of contaminated, dried-up, driller sludge is not re-examined because the climate at the granite site is quite wet compared to that of the salt site and therefore the environment is not suitable for long-term resuspension of dried particulates.

The Driller Exposure Pathway (Case 1) is identical to that described in Section 14.2.1. The waste parcels utilized in the source term are as described in Rechar, Ed. (1993). Waste Disposal Group 1 for the granite repository consists of Waste Parcels 2 through 9; Waste Parcel 1 is excluded. The drill depth for the granite repository is assumed to be 300 m.

The concentrations in the groundwater used for both the Lake Exposure pathway and the Farm Well Pathway are taken from the lower aquifer at a location below the downgradient edge of the repository. The Farm Well scenario takes place approximately 10,000 yr* after repository closure.

* The transport calculations done for the salt and granite sites end at 9500 yr with some variance because of vector-dependent time-stepping. The transport calculations for the tuff site end at 10,000 yr and used vector-independent time-stepping. In the above paragraph and hereafter, this time period is referred to as "approximately 10,000 yr."

14.4 GENII-S: Dosimetry Model for the Safety Assessment

For the 1994 PA, potential doses resulting from exposure to radionuclides hypothetically released from the disposal system repositories were calculated for the exposure scenarios considered (as described in Section 14.2). The principal code for this calculation is the GENII-S code (Leigh et al., 1993).

GENII-S is an amalgamation of the GENII (Napier et al., 1988a, 1988b, 1988c) and SUNS (Campbell et al., 1991) codes. GENII calculates radiation doses to individuals or populations from acute or chronic radionuclide releases to air, water, or soil. It was first developed at Pacific Northwest Laboratories. SUNS is a sensitivity and uncertainty analysis software shell that allows GENII to perform sensitivity and uncertainty analyses. Dose calculations performed by GENII-S follow the ICRP guidelines presented in ICRP Publication 26 (ICRP, 1977) and Publication 30 (ICRP, 1979).

Three types of doses are calculated by GENII-S: (1) the internal effective dose equivalents (EDEs), (2) external dose, and (3) total EDEs.

Internal effective dose equivalents are either committed EDEs or cumulative EDEs. A committed EDE is the dose that is expected to occur over an individual's or a population's lifetime as a result of an intake from ingestion or inhalation of radionuclides for a period of one year. Figure 14-2 is a schematic representation of the extended internal dose expected from an initial exposure. It is referred to as an effective dose equivalent because it is not an actual dose, but rather a prediction of the dose that will occur due to radionuclides present in the individual's body.

In Figure 14-2, *intake* represents a constant rate of radionuclide intake (from inhalation and/or ingestion) and *dose rate* represents the resulting dose rate to tissue or organ. The integral of the dose rate over 50 or 70 years gives the committed dose (i.e., the area under the dose-rate curve) resulting from one year of intake. EDEs for 50- and 70-yr commitment periods are typical for dose calculations. Parameters for these commitment periods are determined by the GENII-S user as data input. The 1994 PA calculates 50-yr dose commitments.

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Figure 14-2. Situation showing committed dose (area under curve) from 1-yr internal intake dose.

1 A cumulative EDE is the dose that is expected over an individual's or a population's average lifetime as a result
 2 of continued intake (greater than one year) of radionuclides. The intake period for cumulative EDE can vary from
 3 greater than one year to the expected lifetime. Although 50-yr and 70-yr EDEs are common, GENII-S accepts any
 4 time period.
 5

6
 7 The external dose calculated by GENII-S is an actual dose that results from exposure to the source for any length
 8 of time. Exposure times are specified in the GENII-S input. The total dose is the whole-body effective dose equivalent (WEDE) representing the sum of the internal and external doses.
 9
 10

11
 12 GENII-S calculates radiation doses resulting from internal and/or external exposure to contaminated air, water,
 13 soil, or to products derived from contaminated air, water, or soil. Data may be entered into the code in one of three
 14 ways. First, a release of radioactive material into the air, surface water, or deep soil may be specified. Given the
 15 release information, GENII-S will estimate the movement of the radioactive material to the exposure location and
 16 calculate the subsequent doses to an individual or population there. Second, the concentration of radionuclides in the
 17 air, surface water, ground water, or surface soil at the exposure location may be specified. In that case, GENII-S will
 18 calculate the subsequent dose to an individual or population there. However, GENII-S does not have the capability to
 19 calculate groundwater transport. Third, the concentration of radionuclides in consumer goods derived from contaminated air, water, or soil may be specified. For example, the radionuclide concentration in milk or drinking water may be given. Given such data, GENII-S will calculate the subsequent dose to an individual or population who consumes the food product(s). Food transfer factors provide information about the magnitude of radionuclides that migrate from soil to plants, as well as to dairy and meat products.
 25
 26

27 The food transfer factors for plant uptake of radionuclides reflect results of recent studies and data compilations.
 28 Many sources were reviewed. The following references formed the basis of this analysis: Adriano et al., 1986;
 29 Coughtrey et al., 1984; Grogan, 1985; IAEA, 1987 (Working Draft); Jackson, 1984; Lawson and Smith, 1985; Miller
 30 et al., 1980; NCRP, 1986; Ng et al., 1982; Romney et al., 1981; Sheppard et al., 1984; US NRC, 1976 (for comparison); and Voilleque et al., 1985.
 33

34 The values in Table 14-1 are based on the dry weight of the plant and soil. Some of the data from which this
 35 table is derived were given as wet crop weight. Where conversions were stated in the literature, their inverses were
 36 used to calculate dry weight. Otherwise, the conversions to dry weight are based on 75% water content. Most, but
 37 not all, values represent the edible fraction of the crop. Data from stable and radioactive elements are used interchangeably. Although there are limited data to support this approach, it is believed that the behavior of the elements is determined primarily by chemical state and that a high degree of disparity is not expected.
 41
 42

43 The variation among researchers on the uptake of the various radionuclides (and stable elements) even within the
 44 same plant group complicates the selection of a definitive value for any given element. Researchers who have compiled previous listings of uptake factors have cautioned that even establishing a range of reasonable factors is difficult because so many physical, chemical, and biological parameters are involved in each analysis. Even so, because of the need for specific values as input to transport codes, the assignment of single numbers is necessary and it is especially important that the relative values of the numeric set be as consistent as possible in spite of uncertainty of the individual values.
 51

52 The extent of the radiological damage to various organs of the human body depends, calculationally, on transfer
 53 factors that determine how much of the ingested contamination is transferred into various organs and on factors called
 54 "internal dose factors." Internal dose factors relate radiation types (γ , β , α) and energies, e.g., from nuclear disintegration to biological effects, measured in units of rem or sieverts (Sv) (1 Sv equals 100 rem). Doses in this report are in units of rem unless indicated otherwise.
 58

59 Internal dose factors are calculated in subroutine INTDF of GENII-S. This subroutine calculates the incremental
 60 organ doses for each year following an initial intake. The detailed procedure is described below.
 61
 62
 63
 64
 65
 66

14. Biosphere Modeling

Table 14-1. Food Transfer Factor Library – (RAP 29-Aug-88) (UPDATED LEACHING FACTORS)

Element	DepVel (m/sec)	Leafy Veg	Root Veg	Fruit	Grain	Beef (day/kg)	Poultry (day/kg)	Milk (day/L)	Egg (day/kg)	Leaching Factor
AM	1.0E-3	2.0E-3	2.0E-3	2.0E-3	2.0E-4	2.0E-5	2.0E-4	3.0E-7	9.0E-3	1.3E-03
SB	1.0E-3	5.0E-2	5.0E-2	5.0E-2	5.0E-2	1.0E-3	6.0E-3	7.5E-4	7.0E-2	4.2E-02
BA	1.0E-3	4.0E-2	4.0E-2	4.0E-2	4.0E-3	5.0E-4	8.1E-4	4.8E-4	1.5E+0	9.5E-05
CD	1.0E-3	2.0E+0	2.0E+0	2.0E+0	6.0E-1	4.0E-4	8.4E-1	1.2E-4	1.0E-1	6.3E-04
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.0E-01
CS	1.0E-3	2.0E-2	2.0E-2	2.0E-2	1.0E-2	3.0E-2	4.4E+0	7.0E-3	4.9E-1	1.1E-03
CE	1.0E-3	4.0E-2	4.0E-2	4.0E-2	4.0E-3	2.0E-3	1.0E-2	4.0E-5	5.0E-3	5.0E-04
CL	1.0E-3	5.0E+1	5.0E+1	5.0E+1	1.0E+0	3.0E-2	3.0E-2	2.0E-2	9.9E-4	8.0E-01
CO	1.0E-3	1.0E-1	1.0E-1	1.0E-1	4.0E-3	2.0E-2	5.0E-1	1.0E-4	1.0E-1	3.0E-02
CM	1.0E-3	2.0E-3	2.0E-3	2.0E-3	2.0E-4	5.0E-3	4.0E-3	3.0E-7	2.0E-3	1.3E-04
EU	1.0E-3	1.0E-2	1.0E-2	1.0E-2	2.0E-3	6.0E-3	4.0E-3	2.0E-5	7.0E-3	5.0E-04
I	1.0E-2	4.0E-1	4.0E-1	4.0E-1	4.0E-1	2.0E-3	1.8E-2	1.2E-2	2.8E+0	0.8
FE	1.0E-3	2.0E-2	2.0E-2	2.0E-2	5.0E-3	2.0E-2	1.5E+0	5.0E-5	1.3E+0	1.8E-02
KR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8
PB	1.0E-3	1.0E-1	1.0E-1	1.0E-1	1.0E-2	4.0E-4	9.9E-4	3.0E-5	9.9E-4	4.5E-04
ND	1.0E-3	1.0E-2	1.0E-2	1.0E-2	1.0E-3	5.0E-3	4.0E-3	2.0E-5	2.0E-4	4.1E-04
NP	1.0E-3	1.0E+0	1.0E+0	1.0E+0	1.0E-1	1.0E-3	4.0E-3	1.0E-5	2.0E-3	3.3E-03
NI	1.0E-3	1.0E-1	1.0E-1	1.0E-1	5.0E-2	2.0E-3	1.0E-3	1.0E-3	1.0E-1	4.6E-03
PD	1.0E-3	3.0E-1	3.0E-1	3.0E-1	5.0E-2	1.0E-3	3.0E-4	5.0E-3	4.0E-3	4.6E-03
PU	1.0E-3	4.0E-4	4.0E-4	4.0E-4	4.0E-5	2.0E-6	1.5E-4	1.0E-7	8.0E-3	1.3E-03
PM	1.0E-3	1.0E-2	1.0E-2	1.0E-2	1.0E-3	5.0E-3	2.0E-3	2.5E-6	2.0E-2	5.0E-04
PA	1.0E-3	5.0E-2	5.0E-2	5.0E-2	2.0E-2	5.0E-3	4.0E-3	2.5E-6	2.0E-3	1.3E-03
RA	1.0E-3	1.0E-1	1.0E-1	1.0E-1	1.0E-2	9.0E-4	9.9E-4	2.0E-4	2.0E-5	5.9E-04
RB	1.0E-3	3.0E-1	3.0E-1	3.0E-1	3.0E-1	1.0E-2	2.0E+0	1.0E-2	3.0E+0	4.4E-03
RU	1.0E-3	2.0E-1	2.0E-1	2.0E-1	2.0E-1	2.0E-3	7.0E-3	6.0E-7	6.0E-3	7.6E-04
SM	1.0E-3	1.0E-2	1.0E-2	1.0E-2	2.0E-3	5.0E-3	4.0E-3	2.0E-5	7.0E-3	4.1E-04
SE	1.0E-3	5.0E-1	5.0E-1	5.0E-1	5.0E-2	1.0E+0	8.5E+0	2.3E-2	9.3E+0	1.7E-02
SR	1.0E-3	2.0E+0	2.0E+0	2.0E+0	2.0E-1	8.0E-4	3.5E-2	1.3E-3	3.0E-1	2.7E-03
TC	1.0E-3	4.0E+1	4.0E+1	4.0E+1	4.0E+1	9.9E-4	3.0E-2	3.0E-4	3.0E+0	0.8
TE	1.0E-3	5.0E+0	5.0E+0	5.0E+0	5.0E-1	7.0E-3	8.5E-2	4.5E-4	5.2E+0	0.8
TH	1.0E-3	4.0E-3	4.0E-3	4.0E-3	4.0E-4	5.0E-3	4.0E-3	2.5E-6	2.0E-3	5.3E-04
SN	1.0E-3	1.0E-1	1.0E-1	1.0E-1	1.0E-2	1.0E-2	9.9E-4	1.0E-3	9.9E-4	2.7E-03
U	1.0E-3	4.0E-3	4.0E-3	4.0E-3	2.0E-4	2.0E-4	1.2E+0	6.0E-4	9.9E-1	1.3E-03
Y	1.0E-3	1.0E-2	1.0E-2	1.0E-2	1.0E-3	1.0E-3	1.0E-2	5.0E-6	2.0E-3	5.0E-04
ZR	1.0E-3	4.0E-2	4.0E-2	4.0E-2	4.0E-2	1.2E-6	6.4E-5	5.5E-7	1.9E-4	5.3E-04

External dose is calculated in the EXTDF subroutine of GENII-S, which is a modification of the shielding code ISOSHL (Engel et al., 1966), using dose conversion factors from DOE/EH-0070 (U.S. DOE, 1988c). Table 14-2 contains the external dose factors for general exposure and for the spherical sample ("5 cm sphere") examined by the driller in the Driller Exposure Pathway (Section 14.2.1).

The following theory supporting the internal dose calculations is presented as general information and background for an understanding of the procedure used in the GENII-S program used for the 1994 PA.

The mean absorbed dose rate on the j th organ (or tissue) $\bar{D}_{R,j}^k$ due to radionuclide k or radiation type R is evaluated. This evaluation involves three primary factors: (1) the activity in source region, Ω irradiating the organ A_Ω , (2) the mean energy emitted by radionuclide k or radiation type R (Δ_R), and (3) the ratio of energy absorbed by the j th organ to energy emitted at the source region Φ_R :

$$\bar{D}_{R,j}^k = A_\Omega(\tau) \cdot \Delta_R \Phi_R \quad (14.2-5)$$

is the mean absorbed dose rate or rate of energy sorption in organ j per unit mass. Because there is more than one type of radiation, a sum over radiation types is performed:

$$\bar{D}_{R,j}^k = A_\Omega(\tau) \left(\sum_R \Delta_R \Phi_R \right). \quad (14.2-6)$$

The activity may also be present in more than one source organ. Therefore, a sum over source regions, Ω , is performed:

$$\bar{D}_{R,j}^k = \sum_\Omega A_\Omega(\tau) \sum_R \Delta_R \Phi_R. \quad (14.2-7)$$

Now the quantity S , the mean absorbed dose rate in organ j per unit of radioactivity in Ω , is defined as

$$S = \sum_R \Delta_R \Phi_R. \quad (14.2-8)$$

Therefore,

$$\bar{D}_{R,j}^k = \sum_\Omega A_\Omega(\tau) S. \quad (14.2-9)$$

The S factor can be written in terms of dose equivalent[†] by inclusion of modifying factors Q_R and N where Q_R is called the quality factor that weights the absorbed dose according to the biological effectiveness of the radiation type producing the dose and N is the product of all other modifying factors. Presently, $N = 1$ is assigned by the ICRP.

[†] The dose equivalent of the point P has been defined by the ICRP (1977) as

$$H(P) = D(P) Q(P) N$$

$D(P)$ is the absorbed dose expressed as

$$D(P) = \lim_{\Delta V \rightarrow P} \left(\frac{\Delta \bar{E}}{\Delta M} \right).$$

where $\Delta \bar{E}$ is the mean energy emitted by the radiation event.

Note: The absorbed dose is an integral quantity that corresponds to the deposition of energy over time. The absorbed dose is considered inadequate for the prediction of health effects that are associated with irradiation of tissue and therefore the modified quantity, dose equivalent, was defined above. The term "dose" is generally used in place of "dose equivalent."

Table 14-2. External Dose Factors for GENII

n	Air Submersion (sv/yr per Bq/m ³)	Water Surface (sv/yr per Bq/L)	DOE/EH-0070 (sv/yr per Bq/m ³)	Buried 0.15 m (sv/yr per Bq/m ³)	Buried 0.5 m (sv/yr per Bq/m ³)	Buried 1.0 m (sv/yr per Bq/m ³)	5 cm Sphere ^a
¹⁴ C	1.41E-11	2.02E-11	0.0E+00	8.89E-19	3.86E-24	3.56E-31	3.18E-18
³⁶ Cl	7.52E-10	1.05E-09	2.1E-16	5.16E-15	1.09E-17	4.80E-21	2.39E-16
⁵⁵ Fe	6.07E-10	8.90E-10	9.8E-13	0.00E+00	0.00E+00	0.00E+00	7.20E-17
⁶⁰ Co	4.31E-06	5.19E-06	1.0E-08	3.83E-10	8.23E-12	4.08E-14	1.13E-12
⁵⁹ Ni	7.37E-10	1.08E-09	1.8E-12	0.00E+00	0.00E+00	0.00E+00	8.74E-17
⁶³ Ni	6.50E-13	9.47E-13	0.0E+00	6.96E-24	4.40E-34	0.00E+00	9.63E-20
⁷⁹ Se	1.05E-11	1.50E-11	0.0E+00	5.17E-19	2.03E-24	1.33E-31	2.30E-18
⁸⁵ Kr	4.84E-09	6.69E-09	1.0E-11	2.11E-13	1.16E-15	8.12E-19	1.38E-15
⁸⁷ Rb	5.51E-11	7.81E-11	0.0E+00	3.08E-17	1.02E-21	5.93E-27	1.66E-13
⁹⁰ Sr	3.51E-10	4.90E-10	0.0E+00	1.28E-15	1.41E-18	3.85E-22	7.49E-13
⁹⁰ Y	1.27E-08	1.74E-08	0.0E+00	3.83E-13	3.52E-15	1.31E-17	1.08E-16
⁹³ Zr	4.83E-13	7.06E-13	0.0E+00	1.35E-24	3.32E-35	0.00E+00	6.88E-20
^{93m} Nb	2.94E-10	4.31E-10	4.5E-12	0.00E+00	0.00E+00	0.00E+00	3.49E-17
⁹⁹ Tc	6.61E-11	9.35E-11	2.8E-15	4.52E-17	2.44E-21	3.90E-26	1.82E-17
¹⁰⁶ Ru	4.15E-07	5.77E-07	9.3E-10	2.36E-11	2.50E-13	1.05E-15	1.20E-13
¹⁰⁷ Pd	2.20E-14	3.23E-14	0.0E+00	0.00E+00	0.00E+00	0.00E+00	2.63E-21
^{113m} Cd	4.10E-10	5.72E-10	0.0E+00	1.76E-15	2.39E-18	7.80E-22	1.27E-16
^{121m} Sn	0.00E+00	0.00E+00	0.0E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
¹²⁵ Sb	8.41E-07	1.20E-06	2.0E-09	4.23E-11	2.51E-13	1.98E-16	2.48E-13
^{125m} Te	2.39E-08	3.46E-08	9.3E-11	1.96E-15	7.23E-20	4.61E-26	4.01E-15
¹²⁶ Sn	4.62E-08	6.54E-08	2.7E-10	3.53E-14	7.97E-20	1.31E-27	1.68E-14
¹²⁹ I	1.55E-08	2.25E-08	9.7E-11	5.72E-19	2.27E-24	1.51E-31	2.62E-15
¹³⁴ Cs	2.93E-06	3.99E-06	7.0E-09	1.77E-10	1.76E-12	4.46E-15	8.54E-13
¹³⁵ Cs	2.36E-11	3.36E-11	0.0E+00	4.52E-18	7.93E-23	4.31E-29	5.83E-18
¹³⁷ Cs	9.84E-07	1.46E-06	2.6E-09	5.33E-11	3.39E-13	2.91E-16	3.03E-13
¹⁴⁴ Ce	2.42E-08	3.32E-08	9.5E-11	7.61E-14	2.77E-18	1.87E-24	8.61E-15
¹⁴⁷ Pm	3.67E-11	5.19E-11	1.8E-14	2.83E-17	9.20E-22	5.75E-28	9.84E-18
¹⁴⁷ Sm	0.00E+00	0.00E+00	0.0E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
¹⁵¹ Sm	8.04E-12	1.18E-11	2.3E-14	1.25E-22	5.74E-31	0.00E+00	1.02E-18
¹⁵² Eu	2.07E-06	2.66E-06	4.9E-09	1.63E-10	3.47E-12	2.05E-14	5.65E-13
¹⁵⁴ Eu	2.12E-06	2.69E-06	5.3E-09	1.63E-10	3.00E-12	1.40E-14	5.91E-13
¹⁵⁵ Eu	7.19E-08	9.96E-08	3.2E-10	1.67E-13	5.34E-18	3.37E-24	2.63E-14

^a Factors were calculated for a 5-cm sphere of material.

Table 14-2. External Dose Factors for GENII (Continued)

n	Air Submersion (sv/yr per Bq/m ³)	Water Surface (sv/yr per Bq/L)	DOE/EH-0070 (sv/yr per Bq/m ³)	Buried 0.15 m (sv/yr per Bq/m ³)	Buried 0.5 m (sv/yr per Bq/m ³)	Buried 1.0 m (sv/yr per Bq/m ³)	5 cm Sphere*
²³⁰ Th	5.11E-10	7.22E-10	4.0E-12	4.90E-16	1.76E-20	1.12E-26	1.43E-16
²²⁶ Ra	6.55E-09	8.94E-09	3.4E-11	2.50E-14	6.04E-18	1.65E-21	2.44E-15
²¹⁰ Pb	2.16E-09	3.08E-09	1.3E-11	1.31E-20	1.12E-35	0.00E+00	4.81E-16
²³² U	4.89E-10	6.96E-10	4.5E-12	5.06E-16	1.86E-20	1.19E-26	4.97E-17
²³² Th	3.49E-10	4.97E-10	2.9E-12	2.92E-16	1.07E-20	6.84E-27	1.12E-16
²²⁸ Ra	5.40E-14	7.92E-14	2.9E-18	9.00E-31	0.00E+00	0.00E+00	7.98E-17
²³⁴ U	3.56E-10	5.11E-10	3.6E-12	2.78E-16	1.02E-20	6.52E-27	6.31E-13
²³⁶ U	2.75E-10	3.99E-10	3.2E-12	3.56E-18	2.64E-26	1.24E-37	7.25E-17
²³⁵ U	1.67E-07	2.28E-07	7.5E-10	8.96E-13	2.43E-16	7.19E-21	4.77E-17
²³¹ Pa	5.54E-08	7.63E-08	1.6E-10	1.68E-12	4.93E-15	1.54E-18	4.59E-15
²³⁷ Np	2.45E-08	3.44E-08	1.4E-10	5.14E-14	7.12E-18	1.99E-22	2.60E-14
²³³ U	4.17E-10	5.77E-10	2.2E-12	1.26E-15	4.65E-20	2.96E-26	8.71E-15
²²⁹ Th	1.01E-07	1.39E-07	4.6E-10	4.33E-13	1.38E-16	4.22E-21	1.27E-13
²³⁸ U	2.43E-10	3.53E-10	2.9E-12	3.11E-18	2.31E-26	1.04E-37	3.27E-15
^{242m} Am	1.03E-09	1.48E-09	1.2E-11	1.14E-15	4.21E-20	2.69E-26	2.10E-16
²⁴² Pu	2.18E-10	3.18E-10	3.0E-12	8.15E-20	2.14E-30	0.00E+00	3.02E-17
²³⁸ Pu	2.72E-10	3.97E-10	3.8E-12	8.71E-20	2.29E-30	0.00E+00	3.70E-17
²⁴⁴ Cm	2.35E-10	3.44E-10	3.7E-12	5.23E-20	1.38E-30	0.00E+00	3.08E-17
²⁴⁴ Pu	1.82E-10	2.66E-10	2.6E-12	9.13E-23	0.00E+00	0.00E+00	2.32E-17
²⁴⁰ Pu	2.62E-10	3.83E-10	3.6E-12	9.66E-20	2.54E-30	0.00E+00	3.63E-17
²⁴⁵ Cm	9.58E-08	1.31E-07	3.8E-10	3.35E-13	1.17E-17	7.32E-24	3.57E-14
²⁴¹ Pu	6.50E-16	9.54E-16	0.0E+00	0.00E+00	0.00E+00	0.00E+00	7.71E-23
²⁴¹ Am	1.87E-08	2.63E-08	1.3E-10	7.18E-17	4.44E-26	1.97E-37	5.84E-15
²⁴⁶ Cm	2.09E-10	3.05E-10	3.2E-12	8.91E-23	0.00E+00	0.00E+00	2.63E-17
²⁴⁷ Cm	7.37E-07	1.02E-06	1.5E-09	3.52E-11	1.93E-13	1.35E-16	2.10E-13
²⁴³ Cm	1.92E-07	2.62E-07	6.4E-10	2.07E-12	1.12E-15	3.55E-20	6.78E-14
²⁴³ Am	4.72E-08	6.55E-08	2.9E-10	1.82E-14	1.77E-19	1.11E-25	1.79E-14
²³⁹ Pu	1.82E-10	2.58E-10	1.7E-12	3.30E-16	1.22E-20	7.75E-27	4.36E-17

* Factors were calculated for a 5-cm sphere of material.

$$S = \sum_R \Delta_R (Q_R \cdot N) \Phi_R. \quad (14.2-10)$$

ICRP (1979), in recommendations on secondary limits, defined the specific effective energy quantity $(SEE)_R$ as

$$(SEE)_R = \sum_R \Delta_R (Q_R \cdot N) \Phi_R. \quad (14.2-11)$$

Therefore, based on this definition

$$\bar{D}_{R,j}^k = \sum_{\Omega} A_{\Omega}(\tau) (SEE)_R \quad (14.2-12)$$

The absorbed dose rate to the organ is from radionuclide R with radiation type j given by $\bar{D}_{R,j}^k$. The absorbed dose rate $\bar{D}_{R,j}^k$ is used to calculate the committed equivalent dose (CED) over the selected commitment period T

$$H_j^k = \int_0^T \bar{D}_{R,j}^k(\tau) \cdot W_R d\tau$$

W_R is the appropriate weighting factor for the type of radiation. The above derivation is taken from Till and Meyer, Eds. (1983). The procedure used in the GENII-S code for the calculation of internal dose follows the method outline above.

In subroutine INTDF of GENII-S, estimates of the dose equivalents in a number of target organs are determined from the activity in a given source organ S . For each type of radiation R , the dose equivalent $H_{j,R}^k$ in target organ j from radionuclide k in source organ (region) S is the product of two factors:

- the total number of nuclear transformations of radionuclide k in source organ S over the period of interest following intake (the committed dose period),
- the energy absorbed per gram in target organ j , modified with a "quality factor" (ICRP, 1977), from radiation of type R per transformation of radionuclide k in source organ.

For each radiation of type R from radionuclide k , the dose equivalent is given by the expression

$$H_{j,R}^k = U_S \cdot 1.6 \cdot 10^{-13} \cdot (SEE)_R \cdot 10^3 \quad (14.2-13)$$

where U_S = the number of transformations of radionuclide k , in source organ S , over the period of integration following intake of the radionuclide (i.e., the commitment period) and the factor 1.6×10^{-13} is the number of joules in 1 MeV. $(SEE)_R$ is the specific effective energy for radiation of type R (in MeV/gm) modified by the quality factor, which is absorbed by organ j from each radionuclide transformation emitted by the source organ. The factor 10^3 converts gm^{-1} to kg^{-1} .

In the general case, for the intake of a mixture of radionuclides, which consist of parents with daughters, the dose in the target organ j from radioactivity emitted from several different source organs is given by

$$H_j = 1.6 \cdot 10^{-10} \cdot \sum_S \sum_k \left[U_S \cdot \sum_R (SEE)_R \right]_k. \quad (14.2-14)$$

The units of dose are in Sv (sieverts). The committed effective dose equivalent (CEDE) is calculated as outlined in ICRP 26 (1977) as

$$CEDE = \sum_j W_j \cdot H_j, \quad (14.2-15)$$

where the factor W_j is the organ weighting factor given in ICRP 26 (1977) and listed below.

The CEDE (as outlined in ICRP 26 (1977)) for the whole body, is given by:

$$CEDE = \sum_j W_j H_j + \text{external dose} \quad (14.2-16)$$

where j is an organ index, W_j is a weighing factor for a particular organ (ICRP, 1977), and H_j is a "dose equivalent" for that same organ. H_j is calculated for the period of integration shown in Figure 14-2, which illustrates conceptually a 50-yr committed dose. H_j also depends on the radiation types and energies from radioactive disintegrations in the body organs. A detailed description of these equations can be found in Volume 1, Hanford Environmental Radiation Dosimetry Software System (Napier et al., 1988a).

For the calculations, the various human organs are weighted as listed below:

Organ:	W_j
gonads	0.25
breast	0.15
red bone marrow	0.12
lung:	0.12
thyroid:	0.03
bone:	0.03
remainder:	0.30

The exposure pathways available in GENII-S are listed in Table 14-3. External radiation doses occur when an individual or population is exposed to (1) contaminated surface soil (groundshine), (2) radionuclide particulates suspended in air (finite or infinite plume), or (3) contaminated non-drinking water sources (bathing, swimming, boating, shoreline activities). Internal radiation doses arise through inhalation or ingestion. Inhalation exposures occur when an individual or population breathes in suspended radionuclide particulates. The particulates can be part of a contaminant plume that is advecting downwind or they can be resuspended particulates that were once deposited on surface soil. Ingestion exposures occur when an individual or population consumes a contaminated food product (drinking water, leafy vegetables, meat or fish that has undergone exposure).

GENII-S input data arise from a variety of sources, some specified by the code, others by the user. Default data are generally not application specific and are contained in a file accessed by the code. They include inventory parameters such as source conversion and soil-source conversion factors, environmental factors addressing absolute humidity, air dispersion conservation flag, deposition velocity/resuspension, leaf resuspension, depth density, soil ingestion, weathering time, animal consumption, animal drinking water, acute fresh forage by season, shore-width factors, swim-water ingested, acute and chronic breathing rates, vegetable production, shore width, and weighting factors for organ doses. Application-specific data must be provided by the code user.

To provide GENII-S with the source term concentrations and input appropriate for LHS sampling capabilities, a CAMCON-linked software tool named PREGENII was applied to compute concentrations of radionuclides for critical pathways, waste types, and scenarios treated in previous performance assessments. This process is represented

Table 14-3. Exposure Pathways for Tuff, Salt, and Granite Disposal Systems Included in 1994 PA

External Exposure	Inhalation Exposure	Ingestion Exposure
Groundshine	Finite Plume	Drinking Water
Finite Plume	Infinite Plume	Leafy Vegetables
Infinite Plume	Resuspension	Root vegetables
Swimming		Grains
Boating		Fruit
Shoreline		Milk
		Beef
		Eggs
		Poultry
		Aquatic Foods
		Soil
		Swimming Water

schematically in Figure 14-3. Additional information such as χ/Q , a measure of air dispersion of contaminated surface soils that is derived from a semi-infinite plume model, can also be supplied. PREGENII can furthermore supply discrete, uniform, normal, or lognormal fits to concentration samples. In the case of normal or lognormal fits, the number of standard deviations from the mean for which significant data can be included can be specified. This feature provides the analyst with flexibility in evaluating the nature or integrity of the data.

A new postprocessor, POSTGENII, was created to transfer output data from GENII-S to CAMDAT files so that the suite of processing packages available in the overall modeling system, CAMCON, could be used so that its capabilities for displaying results are enhanced (see Appendix G).

For example, output data from 36 sample driller calculations performed for the tuff disposal system were transferred from GENII-S to CAMDAT. The purpose of the transfer was to incorporate into the results probabilities of various waste parcels being intercepted by drill bits of varying diameters. At present, this type of information cannot be incorporated into GENII-S input so that its resulting CCDF would reflect these probabilities.

14.4.1 Model for Exposure of a Driller (Case 1)

The first exposure scenario considered involves a worker at the drilling location who is exposed through groundshine and handling of a spherical piece of the waste taken directly from the repository through the drilling operation.

Baseline Data for Exposure of a Driller (Case 1). To estimate groundshine exposure doses, GENII-S requires: (1) the radionuclide concentration in the surface soil, (2) the size of the contaminated area, and (3) the duration of the exposure to the contaminated area. As described previously, the concentrations are calculated by PREGENII. The contaminated area was assumed to be 100 m² except where otherwise noted. Depending on the size of the contaminated area, GENII-S can use either of two external-dose conversion factors, one for a finite source of a given geometry or another for an infinite plane source. In this case, the infinite-plane option was used, representing a more conservative estimate. It was assumed the total exposure time for the driller was one week.

To estimate the exposure resulting from direct handling of a piece of waste, GENII-S requires: (1) the radionuclide concentration in the waste, (2) the size and geometry of the piece of waste, and (3) the length of time the worker handled it. Radionuclide inventories in curies in the waste were given by the WPRD code. Concentrations were estimated by PREGENII, as described previously. The waste was assumed to be spherical, 5 cm in radius. External-dose conversion factors for this geometry were calculated and provided by Bruce Napier (personal communication). A maximum exposure time of one hour was assumed.

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Figure 14-3. Schematic of biosphere transport modeling.

Variables Chosen for Exposure of a Driller (Case 1). The variables required by the GENII-S program for calculation of the dose to the driller are the mud pit exposure area, the external exposure time (hours) for both ground-shine exposure to the mud pit and exposure to an extracted sample, and the nuclide soil concentration in the mud pit and the extracted sample. It was assumed that the radionuclide concentration is identical in both sources, namely the mud pit and the extracted sample. The extracted sample was assumed to have a radius of 5 cm. The external exposure time to the mud pit was taken to be 168 hours. Exposure to the extracted sample was 1 hour. The mud pit area was 100 m². Radionuclide concentrations were assigned distributions based on the results of the WPRD code and PREGENII. In the case of no sampling, deterministic calculations were performed. The deterministic distributions of radionuclides in the mud pit and the extracted sample from the salt, granite, and tuff repositories at 7500-yr intrusion time appear in Table 14-4. The nuclide concentrations are presented as empirical distributions (a range of values) resulting from a sampling process.

14.4.2 Model for Farm-Family Exposure due to a Dried Settling Pond (Case 2a)

This scenario involves exposure of a hypothetical farm family located 2400 m from a dried sludge pit[‡] left by a hypothetical driller. Wind erosion of the dried sludge creates a plume of contaminated material that advects past the farm location. The plume of material is assumed continuous over a 100-yr period before the farm family settles on the land. PREGENII estimated the release of radionuclide particulates into the air at the sludge pit and calculated an air transport parameter, χ/Q . The air transport calculation to the farm, and the radionuclide particulate concentrations in soil and crops at the farm were calculated by GENII-S.

For a point source at the pit, radionuclide particulate concentrations in air at the farm are provided by using a semi-infinite plume model, described earlier. Concentration estimates at the farm are thereby given by the concentration at the sludge pit multiplied by χ/Q (see Equation 14.2-4).

Baseline Data for Farm-Family Exposure due to a Dried Settling Pond (Case 2a). External exposures to the farm family are the result of two processes. The first process involves radionuclide deposition at the farm site during the 100-yr period preceding settlement of the land. The second process involves exposure to suspended radionuclide particulates as the contaminant plume passes the farm. When members of the farm family are outdoors, they will be exposed to both sources. The amount of exposure depends directly on the length of time spent in contact with the source. Assuming steady winds (a worst case), the plume exposure time and the surface-soil exposure time will be the same. The range of values selected for this scenario are discussed in the following paragraphs.

Inhalation doses result from exposure to the contaminant plume, which contains materials from the dried sludge pit as well as materials previously deposited on the farm that were resuspended by the wind. GENII-S contains two codes for predicting resuspension, a mass-loading code and the Anspaugh code. The Anspaugh model was used in these calculations. It requires knowledge of the surface-soil depth subject to resuspension and uses a Gaussian plume model to predict airborne radionuclide concentrations.

The farm family is assumed to ingest plant and root crops grown in plume-contaminated soil and plant crops subject to plume fallout and products from animals fed from feed grown in contaminated soil. GENII-S calculates the radionuclide concentration in these food products. Three transfer mechanisms contribute to the contamination of crops at the farm. The first is seasonal and involves direct deposition onto leaves and fruit as the plume passes. The second involves internal content through root uptake of contaminants deposited on the surface of the soil and subsequently distributed in the upper layers of soil by rain and plowing. The third is similar to the first, but involves the transfer of radionuclides from the surface of the soil to the surface of the crops in the form of dust. To calculate ingestion dose at the farm, GENII-S requires the following input parameters: (1) the growing time; yield; storage time and consumption rates for leafy vegetables, root vegetables, fruits and grains, (2) the dust resuspension factor; deposition velocity, and interception fraction, and (3) the plow depth or surface-soil depth for planting crops.

[‡] Two farm-family scenarios are used in INEL calculations. In one, the family settles 2400 m from a sludge pit (tailings). In the other, they settle 500 m from a dried stockpond. Both grow and consume crops thereafter.

Table 14-4. Case 1 Concentration in Mud Pit at 7500 yr for Driller Intrusion Into Salt, Granite, and Tuff Repositories*

Variable**	Salt and Granite			Tuff	
	Salt (pCi/m ³)	Granite (pCi/m ³)	Distribution	Range of Values (pCi/m ³)	Distribution
¹⁴ C	1.7×10^6	3.9×10^6	Fixed	$1.6 \times 10^6 - 2.3 \times 10^8$	Empirical
³⁶ Cl	4.7×10^4	1.1×10^5	Fixed	$4.6 \times 10^4 - 6.7 \times 10^6$	Empirical
⁵⁹ Ni	3.0×10^5	7.0×10^5	Fixed	$6.6 \times 10^6 - 9.6 \times 10^8$	Empirical
⁷⁹ Se	4.7×10^5	1.1×10^6	Fixed	$4.7 \times 10^5 - 6.8 \times 10^7$	Empirical
⁸⁷ Rb	3.4×10^1	7.0×10^1	Fixed	$3.0 \times 10^1 - 4.4 \times 10^3$	Empirical
⁹³ Zr	2.0×10^7	4.5×10^7	Fixed	$2.0 \times 10^7 - 2.9 \times 10^9$	Empirical
⁹⁹ Tc	1.2×10^7	2.8×10^7	Fixed	$1.3 \times 10^7 - 1.8 \times 10^9$	Empirical
¹⁰⁷ Pd	1.5×10^4	3.4×10^4	Fixed	$1.5 \times 10^4 - 2.2 \times 10^6$	Empirical
¹²⁶ Sn	2.1×10^5	4.9×10^5	Fixed		
¹²⁹ I	3.8×10^4	8.6×10^4	Fixed	$3.8 \times 10^4 - 5.5 \times 10^6$	Empirical
¹³⁵ Cs	2.5×10^5	5.8×10^5	Fixed	$2.4 \times 10^5 - 3.5 \times 10^7$	Empirical
¹⁴⁷ Sm	1.1×10^5	2.5×10^5	Fixed	$2.1 \times 10^5 - 1.6 \times 10^7$	Empirical
²³⁰ Th	6.3×10^5	1.4×10^6	Fixed	$6.6 \times 10^5 - 9.5 \times 10^7$	Empirical
²²⁶ Ra	4.1×10^5	9.5×10^5	Fixed	$4.7 \times 10^5 - 6.8 \times 10^7$	Empirical
²³² Th	8.8×10^4	2.0×10^5	Fixed	$8.8 \times 10^4 - 1.3 \times 10^7$	Empirical
²³⁴ U	9.7×10^6	2.2×10^7	Fixed	$9.8 \times 10^6 - 1.4 \times 10^9$	Empirical
²³⁶ U	3.8×10^5	8.6×10^5	Fixed	$8.7 \times 10^5 - 1.3 \times 10^8$	Empirical
²³⁵ U	4.5×10^4	1.0×10^5	Fixed	$8.4 \times 10^4 - 6.4 \times 10^6$	Empirical
²³¹ Pa	6.3×10^3	1.4×10^4	Fixed	$6.9 \times 10^6 - 8.4 \times 10^8$	Empirical
²³⁷ Np	2.7×10^5	6.2×10^5	Fixed	$2.8 \times 10^5 - 4.0 \times 10^7$	Empirical
²³³ U	7.2×10^7	1.6×10^8	Fixed	$7.2 \times 10^7 - 1.0 \times 10^{10}$	Empirical
²²⁹ Th	3.6×10^7	8.3×10^7	Fixed	$3.7 \times 10^7 - 5.3 \times 10^9$	Empirical
²³⁸ U	1.0×10^3	2.3×10^3	Fixed	$1.0 \times 10^3 - 1.5 \times 10^5$	Empirical
²⁴² Pu	9.9	2.3×10^1	Fixed	$1.2 \times 10^1 - 1.4 \times 10^3$	Empirical
²⁴⁰ Pu	3.0×10^6	7.0×10^6	Fixed	$3.1 \times 10^6 - 4.5 \times 10^8$	Empirical
²⁴⁵ Cm	2.3×10^3	5.4×10^3	Fixed	$2.3 \times 10^3 - 3.3 \times 10^5$	Empirical
²⁴¹ Am	3.0×10^3	7.0×10^3	Fixed	$3.0 \times 10^3 - 4.3 \times 10^5$	Empirical
²⁴⁶ Cm	4.1×10^2	9.5×10^2	Fixed	$4.2 \times 10^2 - 6.0 \times 10^4$	Empirical
²⁴⁷ Cm	3.6×10^3	8.2×10^3	Fixed	$3.6 \times 10^3 - 5.2 \times 10^{-1}$	Empirical
²⁴³ Am	2.3×10^5	5.4×10^5	Fixed	$2.4 \times 10^5 - 3.4 \times 10^7$	Empirical
²³⁹ Pu	3.0×10^6	7.0×10^6	Fixed	$3.0 \times 10^6 - 4.3 \times 10^8$	Empirical

* The concentrations represent the 7500 year intrusion time and Waste Group 1. Other intrusion times not listed.

** Mud pit exposure area is 100 m²; External exposure time is 168 hours

14. Biosphere Modeling

Variables required for the determination of doses to the farm family (Case 2a) include irrigation rates, growing time of crops, yield, storage and consumption rates for leafy vegetables, root vegetables, fruits, grains, and feed for animal products consumed including meat, poultry, and milk. Also required as input are dust resuspension factor, deposition velocity, interception fraction, and contaminated source area. In addition, several GENII-S input parameters were chosen as variables for the 1994 PA sensitivity study. These include (1) plow depth, (2) χ/Q , (3) plume exposure time, (4) inhalation exposure time, (5) soil exposure time, (6) air release terms, and (7) surface-soil depth for the Anspaugh resuspension model. A source for some of these variables was Napier et al. (1988a, 1988b, and 1988c), particularly for data related to food growing and consumption. A selection of these variables with ranges and distributions are shown in Tables 14-5 and 14-6. The radionuclide inventory corresponds to an intrusion event at 1000 yr after repository closure and 10,000 yr after closure.

Table 14-5. Growing Cycle and Consumption Data for GENII-S Case 2a*

	Leafy Vegetables	Root Vegetables	Fruits	Grains	Beef	Poultry
Growing Time (days)	90	90	90	90	45	45
Yield (kg/m ²)	1.5	4	2	0.8	--	--
Holdup Time (days)	0	0	0	0	15	1.0
Consumption Rate (kg/yr)	64	220	330	80	80	30

* This resuspension is applied at the farm site and is unrelated to the resuspension that occurs at either the dried settling pond or stockpond.

Variables Chosen for Farm-Family Exposure due to a Dried Settling Pond (Case 2a). Eight GENII-S input parameters were chosen as sensitivity-study variables for the 1994 PA. They are (1) plow depth, (2) χ/Q value, (3) plume exposure time, (4) inhalation exposure time, (5) soil exposure time, (6) contaminated source area, (7) air release terms and (8) surface-soil depth for the Anspaugh resuspension model. The variables, their ranges, and their distributions are shown in Table 14-6. The radionuclide inventory corresponds to concentrations approximately 10,000 yr after closure.

14.4.3 Model for Farm-Family Exposure due to a Dried Stockpond (Case 2b)

The Farm Stockpond Exposure scenario involves a farm family located 500 m from the dried stockpond left by the rancher (see Case 3). Wind erosion of the dried stockpond creates a plume of contaminated material that travels past the farm location. It is assumed the plume is continuous (i.e., the wind is steady) for a 100-yr period before the farm family settles on the land. The 100-yr period is sufficient for a steady-state concentration to be obtained at the farm site.

GENII-S was used to perform the air transport calculations and determine the radionuclide particulate concentrations in air, soil and crops at the farm. Radionuclide particulate concentrations in the air at the dried stockpond location were calculated by PREGENIL. The concentration at the farm is calculated as the concentration at the dried stockpond multiplied by χ/Q (see Equation 14-2.4).

Baseline Data for Farm-Family Exposure due to a Dried Stockpond (Case 2b). External exposures are the result of two processes (as in Case 2a). The first involves exposure to radionuclides deposited on surface soils outside the land-withdrawal boundary during the 100-yr period preceding settlement of the land. Radiation exposure is modeled assuming a plane source of of 1000 m². The second process involves exposure to suspended radionuclide particulates in the contaminant plume as it passes the farm. For both processes, the amount of exposure varies directly with

Table 14-6. Case 2a Variables for the Safety Assessment

Variable	Range of Values	Distribution
Anspaugh Surface Soil Depth (cm)	25 - 35	Uniform
Plow Depth (cm)	25 - 35	Uniform
CHI/Q (sec/m ³)	$5.659 \times 10^{-7} - 2.647 \times 10^{-6}$	Uniform
Plume Exposure Time (hrs)	$2.628 \times 10^3 - 8.766 \times 10^3$	Uniform
Inhalation Exposure Time (hrs)	$2.628 \times 10^3 - 8.766 \times 10^3$	Uniform
Soil Exposure Time (hrs)	$2.628 \times 10^3 - 8.766 \times 10^3$	Uniform
Contaminated Source Area (m ²)	1000	Fixed
Irrigation Rate	40	Fixed
Direct Resuspension Factor	1.0×10^{-9}	Fixed
Deposition Velocity (m/s)	1.0×10^{-3}	Fixed
Interception Fraction	0.25	Fixed
Home Irrigation Rate (in./yr)	40	Fixed
Home Irrigation Duration (mo.)	6.0	Fixed
Surface Soil Density (kg/m ²)	446.0	Fixed
Nuclide	Release Rate in Air (pCi/yr)	
¹⁴ C	1.1×10^5	Fixed
³⁶ Cl	2.8×10^3	Fixed
⁵⁹ Ni	1.9×10^4	Fixed
⁷⁹ Se	2.9×10^4	Fixed
⁸⁷ Rb	1.8	Fixed
⁹³ Zr	1.2×10^6	Fixed
⁹⁹ Tc	7.3×10^3	Fixed
¹⁰⁷ Pd	9.0×10^2	Fixed
¹²⁶ Sn	1.3×10^4	Fixed
¹²⁹ I	2.3×10^3	Fixed
¹³⁵ Cs	1.5×10^4	Fixed
¹⁴⁷ Sm	6.6×10^3	Fixed
²³⁰ Th	3.8×10^4	Fixed
²²⁶ Ra	2.5×10^4	Fixed
²³² Th	5.3×10^3	Fixed
²³⁴ U	5.9×10^5	Fixed
²³⁶ U	2.2×10^4	Fixed
²³⁵ U	2.7×10^3	Fixed
²³¹ Pa	3.8×10^2	Fixed
²³⁷ Np	1.7×10^4	Fixed
²³³ U	4.4×10^6	Fixed
²²⁹ Th	2.2×10^6	Fixed
²³⁸ U	6.2×10^1	Fixed

Table 14-6. Case 2a Variables for the Safety Assessment (Continued)

Variable	Range of Values	Distribution
^{242}Pu	6.0×10^{-1}	Fixed
^{240}Pu	1.9×10^5	Fixed
^{245}Cm	1.4×10^2	Fixed
^{241}Am	1.8×10^2	Fixed
^{246}Cm	2.5×10^1	Fixed
^{247}Cm	2.2×10^{-4}	Fixed
^{243}Am	1.4×10^4	Fixed
^{239}Pu	1.9×10^5	Fixed

the amount of time spent out of doors. Assuming the plume is continuous, plume exposure time and the surface-soil exposure time will be the same.

Inhalation doses result from exposure to the contaminant plume as it passes the farm and is enriched by radionuclides that were previously deposited and have become resuspended. As in Case 2a, GENII-S's Anspaugh model was used to calculate resuspension loading. It requires knowledge of the surface-soil depth subject to resuspension and uses a Gaussian plume model to predict airborne radionuclide concentrations. For both processes involving inhalation exposures, dose is directly proportional to duration of the exposure. A maximum value of 8,766 hours per year (24 hours per day), was assumed for the calculations.

In order to calculate doses from crop and animal product ingestion, GENII-S calculates the radionuclide concentration in these food products consumed by the farm family. Three transfer mechanisms contribute to the contamination of farm crops. The first mechanism is simple deposition onto crops that are in season when the contaminant plume passes the farm. The second is root uptake of contaminants deposited on the surface of the soil and subsequently distributed throughout the upper soil layers by plowing. The third is the transfer of deposited radionuclides from the surface of the soil to the crops in the form of dust. Transfer to animals is through feed consumed.

GENII-S requires the following input parameters to calculate ingestion dose at the farm: (1) the growing time; yield; storage time; and consumption rate for leafy vegetables, root vegetables, fruits and grains; (2) the dust resuspension factor; deposition velocity; and interception fraction; (3) the plow depth or surface-soil depth for planting crops; and (4) irrigation rates for feed and crops.

Growing time, yield, storage time and consumption rates for leafy vegetables, root vegetables, fruits, grains, animal products, and feed were taken from Napier et al (1988a, 1988b, 1988c). They are the same as shown for Case 2a (Table 14-5). Additional parameters are shown in Table 14-7.

Variables Chosen for Farm-Family Exposure due to a Dried Stockpond (Case 2b). Eight GENII-S input parameters for Case 2b were chosen as variables for the 1994 PA. They are: (1) the plow depth, (2) the CHI/Q value, (3) the plume exposure time, (4) the inhalation exposure time, (5) the soil exposure time, (6) the contaminated source area, (7) the air release terms and (8) surface soil depth for the Anspaugh resuspension model.** The variables, their ranges, and their distributions are shown in Table 14-7.

** This resuspension applies at the farm site and is unrelated to resuspension that occurs at either the dried sludge pit or the stockpond.

14.4.4 Model for a Rancher Exposed to Contaminated Beef (Case 3)

This scenario, which was developed only for the salt site, involves exposure to a rancher who settles at the land-withdrawal boundary at the arrival time for peak radionuclide concentrations via transport through the aquifer, i.e., many centuries after closure. The rancher sinks a shallow well into the aquifer and uses its waters in a stockpond for cattle, which he or she subsequently consumes. GENII-S calculates radionuclide concentrations in the beef and uptake by the rancher through ingestion. The radionuclide pathway to the beef is only through water supplied to the cattle.

Calculations were run for Waste Group 1 release scenario (1993 PA), assuming intrusion into the repository occurs at 1000 yr and from contaminated water approximately 10,000 yr after closure.

Baseline Data for a Rancher Exposed to Contaminated Beef (Case 3). The exposure pathway in this scenario is ingestion of contaminated beef. To model ingestion exposures, GENII-S requires the following information: (1) the rancher's beef consumption rate, (2) the cattle's drinking rate, and (3) the concentration of radionuclides in the stockpond. The beef consumption rate for the rancher was assumed to be 110 kg/yr and the drinking rate for cattle was assumed to be about 26 liters/d. Radionuclide concentrations in the stockpond are discussed below.

Variables Chosen for a Rancher Exposed to Contaminated Beef (Case 3). The radionuclide concentrations in the stockpond were chosen as sensitivity variables for this scenario. They were assigned empirical distributions by PREGENII as described in Section 14.2.3 and as shown in Table 14-8.

Table 14-7. Case 2b Variables for the Safety Assessment

Variable	Range of Values	Distribution
Anspaugh Surface Soil Depth (cm)	25 - 35	Uniform
Plow Depth (cm)	25 - 35	Uniform
CHI/Q (sec/m ³)	2.094×10^{-6} - 1.299×10^{-4}	Uniform
Plume Exposure Time (hrs)	2.628×10^3 - 8.766×10^3	Uniform
Inhalation Exposure Time (hrs)	2.628×10^3 - 8.766×10^3	Uniform
Soil Exposure Time (hrs)	2.628×10^3 - 8.766×10^3	Uniform
Contaminated Source Area (m ²)	1000	Fixed
Nuclide Concentration (pCi/yr)		
²³⁰ Th	1.0×10^{-35} - 8.0×10^1	Empirical
²²⁶ Ra	1.0×10^{-35} - 1.5×10^2	Empirical
²³⁴ U	1.0×10^{-35} - 8.7×10^2	Empirical
²³⁷ Np	1.0×10^{-35} - 6.5	Empirical
²³³ U	1.0×10^{-35} - 5.1×10^2	Empirical
²²⁹ Th	1.0×10^{-35} - 3.4×10^2	Empirical
²⁴⁰ Pu	1.0×10^{-35} - 6.0×10^{-1}	Empirical
²³⁹ Pu	1.0×10^{-35} - 1.9	Empirical

Table 14-8. Case 3 Variables for Rancher Pathway

Groundwater Concentration Nuclide (pCi/l)	Range of Values	Distribution
^{14}C	$1.0 \times 10^{-35} - 8.4 \times 10^{-2}$	Empirical
^{230}Th	$1.0 \times 10^{-35} - 7.6 \times 10^{-2}$	Empirical
^{226}Ra	$1.0 \times 10^{-35} - 2.0 \times 10^{-1}$	Empirical
^{210}Pb	$1.0 \times 10^{-35} - 2.0 \times 10^{-1}$	Empirical
^{234}U	$1.0 \times 10^{-35} - 5.8 \times 10^{-1}$	Empirical
^{237}Np	$1.0 \times 10^{-35} - 5.4 \times 10^{-3}$	Empirical
^{233}U	$1.0 \times 10^{-35} - 5.4 \times 10^{-3}$	Empirical
^{229}Th	$1.0 \times 10^{-35} - 3.9 \times 10^{-1}$	Empirical
^{238}U	$1.0 \times 10^{-35} - 4.2 \times 10^{-3}$	Empirical
^{240}Pu	$1.0 \times 10^{-35} - 1.9 \times 10^{-3}$	Empirical
^{241}Am	$1.0 \times 10^{-35} - 1.3 \times 10^{-5}$	Empirical
^{239}Pu	$1.0 \times 10^{-35} - 6.0 \times 10^{-3}$	Empirical

14.4.5 Model for Lake Exposure Pathway (Case 4)

This scenario considers exposure of a farm family that lives near a lake and whose subsistence depends on the lake water which has been contaminated by a groundwater source. A full description of this scenario appears in Section 14.2.4. Exposure pathways include the following: (1) human drinking water, (2) products from farm animals drinking water and human ingestion of these products including meat, milk, and eggs, (3) ingestion of fruits and vegetables grown on-site utilizing irrigation water, which is untreated, (4) fish from the lake, (5) recreational exposure to the lake including boating and swimming, and (6) external exposure to lake water during fishing activities.

Baseline Data for Lake Exposure (Case 4). To model the exposure pathways for this scenario, GENII-S requires the following information: crop irrigation rates; drinking water consumption; swimming exposure time; inhalation exposure time; boating exposure time; shoreline exposure time, home irrigation rate; home irrigation duration; swim water ingestion rate; vegetable growing time; leaf vegetable, root vegetable, fruit and grain consumption; and beef, poultry, milk, egg, and fish consumption.

Variables Chosen for Lake Exposure Pathway (Case 4). The radionuclide concentrations and required variables for the Lake Exposure Pathway scenario are shown in Table 14-9. The nuclide concentrations are represented as empirical distributions. Because fish consumption was not precisely known, a distribution was selected for this parameter. The remaining parameters were taken as fixed values.

14.4.6 Model for Farm Well Exposure (Case 5)

This scenario considers exposure of a farm family whose location is such that a well can be drilled into the base aquifer that passes below the repository. Enough water is supplied by the well to support the requirements of a modest farm. These include growing and consumption of crops and animal products grown on the farm as well as drinking and irrigation from the well source. The well is located at various distances (see Sections 14.3.1 and 14.3.3) from the repository site. No inhalation or external exposure pathways are considered because the only source of contamination is groundwater. This scenario was used for both the granite and tuff sites.

Table 14-9. Case 4 Variables for the Lake Pathway

Variable	Range of Values	Distribution
Swimming Exposure Time (hr)	10.00	Fixed
Inhalation Exposure Time (hr)	8766	Fixed
Boating Exposure Time (hr)	10.00	Fixed
Shoreline Exposure Time (hr)	210	Fixed
Home Irrigation Rate (in./yr)	40	Fixed
Home Irrigation Duration (mo./yr)	6	Fixed
Swim H ₂ O Ingestion Rate (liters/hr)	0.02	Fixed
Drink Water Consumption (liters/yr)	730	Fixed
Vegetable Growing Time (days)	90	Fixed
Leaf Vegetable Consumption (kg/yr)	64	Fixed
Root Vegetable Consumption (kg/yr)	220	Fixed
Fruit Consumption (kg/yr)	330	Fixed
Grain Consumption (kg/yr)	80	Fixed
Beef Consumption (kg/yr)	40	Fixed
Poultry Consumption (kg/yr)	15	Fixed
Milk Consumption (kg/yr)	310	Fixed
Egg Consumption (kg/yr)	30	Fixed
Fish Consumption (kg/yr)	10-25	Uniform
Nuclide Concentration (pCi/yr)		
¹⁴ C	$7.0 \times 10^{-2} - 8.8 \times 10^1$	Empirical
²³⁰ Th	$6.0 \times 10^{-6} - 1.2 \times 10^0$	Empirical
²²⁶ Ra	$7.0 \times 10^{-6} - 5.7 \times 10^{-1}$	Empirical
²³⁴ U	$5.6 \times 10^{-7} - 3.8 \times 10^1$	Empirical
²³⁷ Np	$5.8 \times 10^{-4} - 8.9 \times 10^{-1}$	Empirical
²³³ U	$5.4 \times 10^{-6} - 8.2 \times 10^{-2}$	Empirical
²²⁹ Th	$5.8 \times 10^{-7} - 7.5 \times 10^0$	Empirical
²³⁸ U	$2.1 \times 10^{-10} - 8.2 \times 10^{-4}$	Empirical
²⁴⁰ Pu	$4.6 \times 10^{-5} - 7.4 \times 10^1$	Empirical
²⁴¹ Am	$1.2 \times 10^{-5} - 2.2 \times 10^2$	Empirical
²³⁹ Pu	$9.7 \times 10^{-5} - 2.3 \times 10^1$	Empirical

Baseline Data for Farm Well Exposure (Case 5). To model the farm well exposure pathway, GENII-S requires the following information: crop irrigation rates; home irrigation rate and duration; drinking water consumption; vegetable growing time; animal growing times; leaf vegetable, root vegetable, fruit and grain consumption; and beef, poultry, milk, and egg consumption, in addition to other data describing the soil and radioactive source characteristics. The radionuclide inventory corresponds to a time approximately 10,000 yr after repository closure.

14. Biosphere Modeling

Variables Chosen for Farm Well Exposure (Case 5). The variables selected for this scenario are listed in Table 14-10. These include radionuclide inventory and associated farm parameters.

Table 14-10. Case 5 Variables for Farm Well Exposure

Variable	Range of Values	Distribution
Home Irrigation Rate (in./yr)	40	Fixed
Home Irrigation Duration (mo./yr)	6	Fixed
Drink Water Consumption (liters/yr)	730	Fixed
Vegetable Growing Time (days)	90	Fixed
Leaf Vegetable Consumption (kg/yr)	64	Fixed
Root Vegetable Consumption (kg/yr)	220	Fixed
Fruit Consumption (kg/yr)	330	Fixed
Grain Consumption (kg/yr)	80	Fixed
Beef Consumption (kg/yr)	40	Fixed
Poultry Consumption (kg/yr)	15	Fixed
Milk Consumption (kg/yr)	310	Fixed
Egg Consumption (kg/yr)	30	Fixed
Nuclide Concentration (pCi/yr)		
^{29}I	$7.8 \times 10^{-28} - 6.4 \times 10^{-4}$	Empirical
^{237}Np	$1.0 \times 10^{-35} - 5.6 \times 10^{-8}$	Empirical
^{231}Pa	$1.0 \times 10^{-35} - 2.7 \times 10^{-9}$	Empirical
^{239}Pu	$1.0 \times 10^{-35} - 6.9 \times 10^{-13}$	Empirical
^{79}Se	$1.0 \times 10^{-35} - 1.0 \times 10^{-10}$	Empirical
^{99}Tc	$6.0 \times 10^{-25} - 3.9 \times 10^{-1}$	Empirical
^{233}U	$1.0 \times 10^{-35} - 1.4 \times 10^{-10}$	Empirical
^{234}U	$1.0 \times 10^{-35} - 4.4 \times 10^{-8}$	Empirical
^{235}U	$1.0 \times 10^{-35} - 1.7 \times 10^{-13}$	Empirical
^{236}U	$1.0 \times 10^{-35} - 4.2 \times 10^{-11}$	Empirical
^{238}U	$1.0 \times 10^{-35} - 1.4 \times 10^{-16}$	Empirical

14.5 Numerical Results of the 1994 INEL Safety Assessment

The 50-year committed dose equivalent was calculated for the exposure scenarios described above.

14.5.1 Results: Exposure of a Driller (Case 1)

GENII-S was used to analyze the scenario of the driller exposed to waste brought to the surface during the drilling operation. Two intrusion times were considered for the salt disposal system; one intrusion time was considered for the granite disposal system. Waste Disposal Group 1 for the salt included waste parcels 1, 4, 5, 6, 7, 8, and 9; for the granite, the waste parcels were 2, 3, 4, 5, 6, 7, 8, and 9. (See Rechard, Ed., 1993, Chapter 4 for a discussion of the waste disposal groups). Results are given in Table 14-11 for the salt disposal system at 125 yr. Table 14-12 provides results for both the salt and granite disposal systems.

Table 14-11. Doses to Driller for Salt Disposal System at 125 Yr Intrusion, Waste Disposal Group 1

Waste Parcel ID	Ground Shine Exposure (rem)	Sample Exposure (rem)	Total
WP 1	1.39×10^{-6}	3.26×10^{-7}	1.71×10^{-6}
WP 4	2.89×10^{-7}	8.06×10^{-8}	3.70×10^{-7}
WP 5	5.65×10^{-6}	1.29×10^{-6}	6.94×10^{-6}
WP 6	3.79×10^{-7}	9.87×10^{-8}	4.78×10^{-7}
WP 7	6.09×10^{-7}	2.69×10^{-6}	3.30×10^{-6}
WP 8	9.21×10^{-6}	2.51×10^{-6}	1.17×10^{-5}
WP 9	1.06×10^{-5}	1.52×10^{-6}	1.21×10^{-5}

Table 14-12. Doses to Driller for Salt and Granite Disposal Systems at 7500-Yr Intrusion for Waste Disposal Group 1

Waste Parcel	Salt		Granite		Total Salt	Total Granite
	Groundshine Exposure	Sample Exposure	Groundshine Exposure	Sample Exposure		
1	3.70×10^{-8}	5.55×10^{-9}	n/a	n/a	4.26×10^{-8}	n/a
2	n/a	n/a	4.12×10^{-9}	1.07×10^{-9}	n/a	5.19×10^{-9}
3	n/a	n/a	9.89×10^{-9}	8.65×10^{-10}	n/a	1.08×10^{-8}
4	1.79×10^{-9}	6.45×10^{-11}	4.12×10^{-9}	1.48×10^{-10}	1.85×10^{-9}	4.27×10^{-9}
5	8.06×10^{-9}	4.30×10^{-9}	1.85×10^{-7}	9.89×10^{-9}	1.24×10^{-8}	1.17×10^{-8}
6	2.51×10^{-9}	1.18×10^{-10}	5.77×10^{-9}	2.72×10^{-10}	2.63×10^{-9}	2.90×10^{-9}
7	1.72×10^{-7}	4.84×10^{-9}	3.95×10^{-7}	1.11×10^{-8}	1.77×10^{-9}	5.1×10^{-7}
8	1.97×10^{-7}	3.04×10^{-9}	4.53×10^{-7}	7.00×10^{-9}	2.0×10^{-7}	4.60×10^{-7}
9	9.67×10^{-9}	3.22×10^{-9}	2.22×10^{-8}	7.41×10^{-9}	1.29×10^{-8}	2.96×10^{-8}

14.5.2 Results: Farm-Family Exposure due to a Dried Settling Pond (Case 2a)

GENII-S was used to analyze the scenario of the farm family exposed to a contaminant plume originating from the dried settling pond left. Waste Disposal Group 1 was considered.

Results of these calculations for the salt disposal system appear in Tables 14-13 and 14-14.

Table 14-13. Farm Pathway Doses (rem) by Organ (Case 2a) for Salt Disposal System

Waste Parcel ID	Bone Surface		Red Marrow		Liver		Annual EDE	
	Mean	Max	Mean	Max	Mean	Max	Mean	Max
WP 1	1.7×10^{-5}	3.8×10^{-5}	1.3×10^{-6}	3.1×10^{-6}	1.1×10^{-7}	2.5×10^{-7}	1.5×10^{-6}	3.5×10^{-6}
WP 4	2.0×10^{-7}	4.6×10^{-7}	1.5×10^{-8}	3.5×10^{-8}	3.3×10^{-8}	7.6×10^{-8}	1.8×10^{-8}	4.2×10^{-8}
WP 5	5.9×10^{-5}	1.4×10^{-4}	4.6×10^{-6}	1.0×10^{-5}	1.0×10^{-5}	2.4×10^{-5}	5.5×10^{-6}	1.3×10^{-5}
WP 6	9.1×10^{-7}	2.1×10^{-6}	7.2×10^{-8}	1.6×10^{-7}	1.0×10^{-7}	2.4×10^{-7}	6.5×10^{-8}	1.5×10^{-7}
WP 7	1.3×10^{-5}	3.1×10^{-5}	1.0×10^{-6}	2.4×10^{-6}	2.3×10^{-6}	5.4×10^{-6}	1.3×10^{-6}	3.0×10^{-6}
WP 8	2.8×10^{-6}	6.4×10^{-6}	2.2×10^{-7}	5.0×10^{-7}	3.0×10^{-7}	7.0×10^{-7}	1.9×10^{-7}	4.4×10^{-7}
WP 9	9.5×10^{-6}	2.2×10^{-5}	7.4×10^{-7}	1.7×10^{-6}	1.5×10^{-6}	3.6×10^{-6}	8.0×10^{-7}	1.9×10^{-7}

Table 14-14. Farm Pathway Doses (rem) by Radionuclide (Case 2a) for Salt Disposal System

Waste Parcel ID	¹⁴ C		³⁶ Cl		⁵⁹ Ni		⁷⁹ Se	
	Mean	Max	Mean	Max	Mean	Max	Mean	Max
WP 1	9.2×10^{-12}	1.5×10^{-11}	3.2×10^{-13}	5.3×10^{-13}	1.9×10^{-14}	3.4×10^{-14}	3.7×10^{-11}	6.1×10^{-11}
WP 4	4.7×10^{-17}	7.6×10^{-17}					5.5×10^{-12}	8.9×10^{-12}
WP 5	1.1×10^{-11}	1.8×10^{-11}	2.6×10^{-13}	4.1×10^{-13}	1.0×10^{-12}	1.8×10^{-12}	1.0×10^{-10}	1.6×10^{-10}
WP 6								
WP 7					2.0×10^{-14}	3.6×10^{-14}		
WP 8					1.2×10^{-13}	2.1×10^{-13}	4.2×10^{-12}	6.8×10^{-12}
WP 9					3.5×10^{-13}	6.2×10^{-13}	1.5×10^{-11}	2.4×10^{-11}
	⁸⁷ Rb		⁹³ Zr		⁹⁹ Tc		¹⁰⁷ Pd	
	Mean	Max	Mean	Max	Mean	Max	Mean	Max
WP 1	7.4×10^{-17}	1.2×10^{-16}	3.9×10^{-11}	8.5×10^{-11}	3.0×10^{-13}	4.9×10^{-13}	4.5×10^{-15}	1.0×10^{-16}
WP 4	1.2×10^{-17}	2.0×10^{-17}	7.1×10^{-13}	1.6×10^{-12}	5.8×10^{-12}	9.4×10^{-12}	8.6×10^{-16}	1.9×10^{-15}
WP 5			1.1×10^{-11}	2.5×10^{-11}	1.0×10^{-10}	1.7×10^{-10}	1.1×10^{-13}	2.5×10^{-13}
WP 6								
WP 7	3.1×10^{-17}	5.1×10^{-17}	3.1×10^{-11}	6.8×10^{-11}	1.1×10^{-10}	1.8×10^{-10}	6.6×10^{-14}	1.4×10^{-13}
WP 8			3.5×10^{-11}	7.7×10^{-11}	3.2×10^{-10}	5.3×10^{-10}	1.8×10^{-13}	3.9×10^{-13}
WP 9			3.0×10^{-11}	6.5×10^{-11}	1.5×10^{-11}	2.4×10^{-11}	1.9×10^{-13}	4.0×10^{-13}
	¹²⁶ Sn		¹²⁹ I		¹³⁵ Cs		¹⁴⁷ Sm	
	Mean	Max	Mean	Max	Mean	Max	Mean	Max
WP 1	1.7×10^{-12}	3.0×10^{-12}	4.6×10^{-11}	7.4×10^{-11}	1.1×10^{-12}	1.8×10^{-12}	1.7×10^{-10}	3.9×10^{-10}
WP 4	4.8×10^{-13}	8.3×10^{-13}	4.8×10^{-12}	7.9×10^{-12}	7.8×10^{-14}	1.3×10^{-13}	2.1×10^{-15}	4.9×10^{-15}
WP 5	1.8×10^{-11}	3.2×10^{-11}	1.2×10^{-10}	2.0×10^{-10}	4.8×10^{-12}	7.7×10^{-12}	6.1×10^{-18}	1.4×10^{-17}
WP 6								
WP 7	4.7×10^{-11}	8.2×10^{-11}			6.1×10^{-12}	9.9×10^{-12}	5.6×10^{-14}	1.3×10^{-13}
WP 8	4.9×10^{-11}	8.6×10^{-11}	2.8×10^{-13}	4.5×10^{-13}	1.6×10^{-11}	2.6×10^{-11}	2.2×10^{-14}	5.0×10^{-14}
WP 9	4.3×10^{-11}	7.4×10^{-11}			3.8×10^{-11}	6.3×10^{-11}	1.9×10^{-16}	4.4×10^{-16}
	²³⁰ Th		²²⁶ Ra		²³² Th		²³⁴ U	
	Mean	Max	Mean	Max	Mean	Max	Mean	Max
WP 1	3.3×10^{-9}	7.6×10^{-9}	1.5×10^{-10}	2.8×10^{-10}	2.1×10^{-9}	4.8×10^{-9}	2.6×10^{-8}	6.0×10^{-8}
WP 4	1.3×10^{-11}	2.9×10^{-11}	1.7×10^{-13}	3.1×10^{-13}	7.1×10^{-16}	1.7×10^{-15}	1.1×10^{-10}	2.4×10^{-10}
WP 5	2.1×10^{-9}	4.7×10^{-9}	6.6×10^{-11}	1.2×10^{-10}	7.1×10^{-15}	1.7×10^{-14}	1.7×10^{-8}	3.9×10^{-8}
WP 6	6.7×10^{-11}	1.5×10^{-10}	2.7×10^{-12}	5.1×10^{-12}	3.2×10^{-17}	7.3×10^{-17}	5.3×10^{-10}	1.2×10^{-9}
WP 7	2.7×10^{-9}	6.3×10^{-9}	3.9×10^{-11}	7.4×10^{-11}	2.3×10^{-16}	5.2×10^{-16}	2.1×10^{-8}	4.9×10^{-8}
WP 8	2.5×10^{-11}	5.5×10^{-11}	1.1×10^{-12}	2.2×10^{-12}	6.3×10^{-17}	1.4×10^{-16}	1.9×10^{-10}	4.4×10^{-10}
WP 9	1.5×10^{-10}	3.4×10^{-10}	5.5×10^{-12}	1.1×10^{-11}	2.2×10^{-9}	5.0×10^{-9}	1.1×10^{-9}	2.4×10^{-9}

Table 14-14. Farm Pathway Doses (rem) by Radionuclide (Case 2a) for Salt Disposal System (Continued)

Waste Parcel ID	²³⁶ U		²³⁵ U		²³¹ Pa		²³⁷ Np	
	Mean	Max	Mean	Max	Mean	Max	Mean	Max
WP 1	9.2×10^{-10}	2.2×10^{-9}	1.1×10^{-10}	2.6×10^{-10}	1.2×10^{-10}	2.8×10^{-10}	3.9×10^{-9}	8.8×10^{-9}
WP 4	2.1×10^{-10}	4.8×10^{-10}	4.9×10^{-11}	1.1×10^{-10}	5.6×10^{-11}	1.2×10^{-10}	7.4×10^{-10}	1.7×10^{-9}
WP 5	2.1×10^{-9}	4.8×10^{-9}	1.5×10^{-10}	3.5×10^{-10}	1.6×10^{-10}	3.5×10^{-10}	5.1×10^{-8}	1.2×10^{-7}
WP 6	7.1×10^{-12}	1.6×10^{-11}	2.7×10^{-12}	6.2×10^{-12}	2.9×10^{-12}	6.4×10^{-12}	2.0×10^{-8}	4.4×10^{-8}
WP 7	8.8×10^{-11}	2.0×10^{-10}	8.6×10^{-12}	2.0×10^{-11}	6.6×10^{-12}	1.4×10^{-11}	4.4×10^{-9}	1.0×10^{-8}
WP 8	2.0×10^{-11}	4.7×10^{-11}	7.4×10^{-12}	1.7×10^{-11}	7.8×10^{-12}	1.7×10^{-11}	6.2×10^{-8}	1.4×10^{-7}
WP 9	6.7×10^{-11}	1.5×10^{-10}	1.4×10^{-11}	3.2×10^{-11}	1.4×10^{-8}	3.2×10^{-8}	2.7×10^{-8}	6.2×10^{-8}
Waste Parcel ID	²³³ U		²²⁹ Th		²³⁸ U		²⁴² Pu	
	Mean	Max	Mean	Max	Mean	Max	Mean	Max
WP 1	1.9×10^{-7}	4.6×10^{-7}	1.3×10^{-6}	3.0×10^{-6}	2.4×10^{-12}	5.7×10^{-12}	5.8×10^{-14}	1.3×10^{-13}
WP 4	4.2×10^{-12}	9.7×10^{-12}	1.6×10^{-13}	3.7×10^{-13}	8.6×10^{-13}	2.0×10^{-12}	1.3×10^{-11}	2.9×10^{-11}
WP 5	9.0×10^{-11}	2.0×10^{-10}	3.1×10^{-12}	7.2×10^{-12}	2.4×10^{-9}	5.7×10^{-9}	3.3×10^{-8}	7.6×10^{-8}
WP 6	1.4×10^{-10}	3.2×10^{-10}	1.2×10^{-10}	2.6×10^{-10}	1.4×10^{-13}	3.2×10^{-13}	8.8×10^{-12}	2.0×10^{-11}
WP 7	1.1×10^{-11}	2.6×10^{-11}	7.6×10^{-13}	1.8×10^{-12}	3.6×10^{-10}	8.3×10^{-10}	9.7×10^{-10}	2.3×10^{-9}
WP 8	2.5×10^{-10}	5.8×10^{-10}	8.2×10^{-12}	1.9×10^{-11}	1.3×10^{-10}	3.0×10^{-10}	1.1×10^{-11}	2.5×10^{-11}
WP 9	1.4×10^{-9}	3.4×10^{-9}	8.7×10^{-9}	1.9×10^{-8}	1.1×10^{-10}	2.5×10^{-10}	5.2×10^{-10}	1.2×10^{-9}
Waste Parcel ID	²⁴⁰ Pu		²⁴⁵ Cm		²⁴¹ Am		²⁴⁶ Cm	
	Mean	Max	Mean	Max	Mean	Max	Mean	Max
WP 1	1.9×10^{-8}	4.6×10^{-8}	2.3×10^{-11}	5.3×10^{-11}	2.9×10^{-11}	6.5×10^{-11}	4.1×10^{-12}	9.2×10^{-12}
WP 4	4.2×10^{-9}	9.7×10^{-9}	1.1×10^{-13}	2.5×10^{-13}	1.6×10^{-12}	3.6×10^{-12}	4.6×10^{-15}	1.0×10^{-14}
WP 5	5.9×10^{-8}	1.4×10^{-7}			1.2×10^{-9}	2.6×10^{-9}		
WP 6	8.8×10^{-9}	2.0×10^{-8}			2.4×10^{-13}	5.1×10^{-13}		
WP 7	3.6×10^{-7}	8.5×10^{-7}	5.2×10^{-12}	1.2×10^{-12}	7.9×10^{-11}	1.8×10^{-10}	2.6×10^{-14}	5.8×10^{-14}
WP 8	2.3×10^{-8}	5.5×10^{-8}			6.6×10^{-10}	1.5×10^{-9}		
WP 9	1.9×10^{-7}	4.6×10^{-7}	2.6×10^{-10}	5.8×10^{-10}	5.3×10^{-10}	1.2×10^{-9}	2.0×10^{-11}	4.5×10^{-11}
Waste Parcel ID	²⁴⁷ Cm		²⁴³ Am		²³⁹ Pu		²⁴⁴ Pu	
	Mean	Max	Mean	Max	Mean	Max	Mean	Max
WP 1	3.3×10^{-17}	7.6×10^{-17}	2.2×10^{-9}	5.1×10^{-9}	1.9×10^{-8}	4.6×10^{-8}	2.4×10^{-18}	5.5×10^{-18}
WP 4			4.4×10^{-11}	9.8×10^{-11}	1.3×10^{-8}	3.0×10^{-8}		
WP 5			2.7×10^{-7}	6.0×10^{-7}	5.0×10^{-6}	1.2×10^{-5}		
WP 6			2.7×10^{-7}	6.0×10^{-10}	3.7×10^{-8}	8.5×10^{-8}		
WP 7	8.5×10^{-20}	2.0×10^{-19}	4.0×10^{-10}	8.8×10^{-10}	9.1×10^{-7}	2.1×10^{-6}		
WP 8			4.6×10^{-9}	1.0×10^{-8}	1.0×10^{-7}	2.3×10^{-7}		
WP 9			9.3×10^{-8}	2.1×10^{-7}	4.7×10^{-7}	1.1×10^{-6}		

14.5.3 Results: Farm-Family Exposure due to a Dried Stockpond (Case 2b)

GENII-S was used to analyze the scenario of the farm family exposed to a contaminant plume originating from the dried stockpond left by the rancher. One well-withdrawal time, approximately 10,000 yr, was considered for Waste Disposal Group 1. (Peak concentrations occur at 10,000 yr at the land-withdrawal boundary.)

Results of these calculations for the salt disposal system are given in Tables 14-15 and 14-16.

Table 14-15. Farm Stockpond Pathway (Case 2b) Dose (rem) by Organ

Organ	Mean	Max
Lung	1.8×10^{-14}	1.4×10^{-13}
Stomach	5.1×10^{-14}	3.1×10^{-13}
Small Intestine	1.0×10^{-13}	5.9×10^{-13}
UL Intestine	5.1×10^{-13}	2.9×10^{-12}
LL Intestine	1.5×10^{-12}	8.6×10^{-12}
Bone Surface	1.1×10^{-10}	1.1×10^{-9}
Red Marrow	8.9×10^{-12}	8.7×10^{-11}
Testes	3.0×10^{-14}	1.6×10^{-13}
Ovaries	3.0×10^{-14}	1.6×10^{-13}
Muscle	1.8×10^{-14}	1.4×10^{-13}
Thyroid	1.8×10^{-14}	1.4×10^{-13}
Liver	2.6×10^{-13}	2.0×10^{-12}
Spleen	3.5×10^{-15}	4.4×10^{-14}
Ingestion	4.6×10^{-12}	4.4×10^{-11}
Internal	4.6×10^{-12}	4.4×10^{-11}
External	3.7×10^{-18}	3.7×10^{-17}
Annual	4.6×10^{-12}	4.4×10^{-11}

Table 14-16. Farm Stockpond Pathway (Case 2b) Dose (rem) by Radionuclide

Radionuclide	Mean	Max
^{226}Ra	3.2×10^{-13}	3.9×10^{-12}
^{230}Th	1.3×10^{-13}	1.2×10^{-12}
^{234}U	6.6×10^{-14}	5.5×10^{-13}
^{237}Np	6.5×10^{-14}	8.3×10^{-13}
^{233}U	4.3×10^{-14}	4.6×10^{-13}
^{229}Th	3.8×10^{-12}	4.2×10^{-11}
^{240}Pu	1.3×10^{-16}	2.0×10^{-15}
^{239}Pu	4.5×10^{-16}	7.4×10^{-15}

14.5.4 Results: A Rancher Exposed to Contaminated Beef (Case 3)

Calculations were run for Waste Group 1 at the salt site, assuming intrusion into the repository occurs at approximately 10,000 yr.

Results are given in Tables 14-17 and 14-18.

Table 14-17. Rancher Pathway Doses by (rem) Organ (Case 3)

Intrusion Location	Bone Surface		Red Marrow		Liver		Annual EDE	
	Mean	Max	Mean	Max	Mean	Max	Mean	Max
Site 1	1.6×10^{-5}	4.1×10^{-4}	1.2×10^{-6}	3.3×10^{-5}	2.7×10^{-7}	5.4×10^{-6}	6.7×10^{-7}	1.7×10^{-5}
Site 2	1.1×10^{-8}	2.0×10^{-7}	8.0×10^{-10}	1.4×10^{-8}	2.3×10^{-9}	5.9×10^{-8}	7.5×10^{-10}	1.6×10^{-8}
Site 3	3.7×10^{-11}	8.1×10^{-10}	2.9×10^{-12}	6.4×10^{-11}	4.5×10^{-13}	7.7×10^{-12}	1.6×10^{-12}	3.3×10^{-11}

Table 14-18. Rancher Pathway Doses (rem) by Radionuclide (Case 3)

Intrusion Location	Site 1		Site 2		Site 3	
Radionuclide	Mean	Max	Mean	Max	Mean	Max
^{230}Th	1.5×10^{-8}	3.4×10^{-7}	5.1×10^{-15}	9.1×10^{-14}	4.1×10^{-14}	8.1×10^{-13}
^{226}Ra	1.2×10^{-8}	3.9×10^{-7}	1.2×10^{-10}	3.9×10^{-9}	2.0×10^{-14}	5.4×10^{-13}
^{210}Pb	5.2×10^{-8}	1.3×10^{-6}	5.2×10^{-10}	1.3×10^{-8}	8.0×10^{-14}	1.8×10^{-12}
^{234}U	3.2×10^{-10}	1.1×10^{-8}	1.1×10^{-12}	3.6×10^{-11}	6.2×10^{-16}	1.1×10^{-14}
^{237}Np	3.5×10^{-9}	8.4×10^{-8}	2.1×10^{-12}	4.9×10^{-11}	6.9×10^{-15}	1.3×10^{-13}
^{233}U	3.0×10^{-10}	5.8×10^{-9}	6.9×10^{-17}	8.7×10^{-16}	6.3×10^{-16}	9.2×10^{-15}
^{229}Th	5.3×10^{-7}	1.6×10^{-5}	1.2×10^{-13}	2.3×10^{-12}	1.3×10^{-12}	3.0×10^{-11}
^{238}U	2.4×10^{-12}	9.5×10^{-11}	1.4×10^{-14}	5.4×10^{-13}	5.4×10^{-18}	9.0×10^{-17}
^{240}Pu	1.9×10^{-14}	5.5×10^{-13}	1.2×10^{-21}	1.9×10^{-20}	3.7×10^{-20}	1.0×10^{-18}
^{241}Am	1.4×10^{-13}	3.2×10^{-12}	5.5×10^{-15}	1.2×10^{-13}	1.1×10^{-19}	1.8×10^{-18}
^{239}Pu	9.5×10^{-14}	2.5×10^{-12}	4.5×10^{-21}	7.0×10^{-20}	1.7×10^{-19}	4.3×10^{-18}

14.5.5 Results: Lake-Farm Family Exposure (Case 4)

GENII-S was used to analyze the pathway scenario of the farm family exposed to the usage of a nearby lake for water, irrigation of crops, and recreational purposes. The results of this calculation are given in Tables 14-19 through 14-22 for these cases; the radionuclide inventory corresponds to about 10,000 yr post-closure.

Table 14-19. Dose (rem) by Organ for Lake Scenario Exposure with Dilution for Granite Disposal System

Organ	Mean	Max
Lung	2.0×10^{-12}	1.6×10^{-11}
Stomach	2.2×10^{-12}	1.6×10^{-11}
Small Intestine	2.4×10^{-12}	1.6×10^{-11}
UL Intestine	4.1×10^{-12}	1.8×10^{-11}
LL Intestine	8.6×10^{-12}	4.6×10^{-11}
Bone Surface	4.2×10^{-10}	2.7×10^{-9}
Red Marrow	3.6×10^{-11}	2.2×10^{-10}
Testes	4.3×10^{-12}	2.9×10^{-11}
Ovaries	4.3×10^{-12}	2.8×10^{-11}
Muscle	2.1×10^{-12}	1.6×10^{-11}
Thyroid	2.0×10^{-12}	1.6×10^{-11}
Kidneys	4.9×10^{-14}	8.6×10^{-13}
Liver	1.7×10^{-11}	1.1×10^{-10}
Spleen	1.1×10^{-15}	9.6×10^{-15}
Ingestion	2.1×10^{-11}	1.2×10^{-10}
Internal	2.1×10^{-11}	1.2×10^{-10}
External	1.1×10^{-19}	6.6×10^{-19}
Annual	2.1×10^{-11}	1.2×10^{-10}

Table 14-20. Dose (rem) by Radionuclide for Lake Scenario Exposure with Dilution for Granite Disposal System

Radionuclide	Mean	Max
^{14}C	2.0×10^{-12}	1.6×10^{-11}
^{230}Th	9.7×10^{-14}	8.6×10^{-13}
^{226}Ra	1.0×10^{-13}	9.9×10^{-13}
^{234}U	1.7×10^{-14}	3.3×10^{-13}
^{237}Np	1.3×10^{-11}	9.2×10^{-11}
^{233}U	3.5×10^{-16}	2.2×10^{-15}
^{229}Th	3.6×10^{-12}	4.2×10^{-11}
^{238}U	1.3×10^{-18}	2.7×10^{-17}
^{240}Pu	9.9×10^{-13}	8.6×10^{-12}
^{241}Am	4.6×10^{-13}	3.7×10^{-12}
^{239}Pu	3.7×10^{-13}	2.9×10^{-12}

Table 14-21. Well Extraction Dose (rem) by Organ for Granite Disposal System

Organ	Mean	Max
Lung	2.1×10^{-4}	1.4×10^{-3}
Stomach	5.7×10^{-4}	2.4×10^{-3}
Small Intestine	1.1×10^{-3}	5.5×10^{-3}
UL Intestine	5.5×10^{-3}	3.1×10^{-2}
LL Intestine	1.7×10^{-2}	9.5×10^{-2}
Bone Surface	3.2	3.0×10^{-1}
Red Marrow	2.5×10^{-1}	2.3
Testes	4.3×10^{-2}	4.2×10^{-1}
Ovaries	4.2×10^{-2}	4.1×10^{-1}
Muscle	2.1×10^{-4}	1.4×10^{-3}
Thyroid	2.1×10^{-4}	1.4×10^{-3}
Kidneys	2.2×10^{-4}	4.8×10^{-3}
Liver	5.4×10^{-1}	5.3
Spleen	1.2×10^{-6}	1.3×10^{-5}
Ingestion	1.7×10^{-1}	1.6
Internal	1.7×10^{-1}	1.6
Annual	1.7×10^{-1}	1.6

Table 14-22. Well Extraction Dose (rem) by Radionuclide for Granite Disposal System

Radionuclide	Mean	Max
^{14}C	1.8×10^{-4}	1.2×10^{-3}
^{230}Th	1.2×10^{-4}	1.3×10^{-3}
^{226}Ra	9.8×10^{-5}	1.1×10^{-3}
^{234}U	8.4×10^{-5}	1.9×10^{-3}
^{237}Np	1.7×10^{-3}	1.0×10^{-2}
^{233}U	4.2×10^{-7}	4.0×10^{-6}
^{229}Th	4.5×10^{-3}	5.5×10^{-2}
^{238}U	1.6×10^{-9}	3.7×10^{-8}
^{240}Pu	9.3×10^{-4}	7.8×10^{-3}
^{241}Am	1.6×10^{-1}	1.6
^{239}Pu	3.4×10^{-4}	2.2×10^{-3}

14.5.6 Results: Exposure of Driller at Tuff Site

GENII-S was used to analyze the scenario of the driller exposed to waste brought to the surface during drilling operations for a 7500-yr intrusion time. Results are provided in Table 14-23.

Table 14-23. Committed Total Doses to Driller at Tuff Site, Horizontal Emplacement

Source	Total Exposure (rem)	
	Mean	Max
WP101	2.5×10^{-6}	2.2×10^{-5}
WP102	9.6×10^{-6}	1.3×10^{-4}
WP103	4.1×10^{-6}	6.5×10^{-5}
WP104	4.6×10^{-6}	3.4×10^{-5}
WP105	7.3×10^{-6}	8.9×10^{-5}
WP106	1.1×10^{-7}	1.6×10^{-6}
WP107	9.4×10^{-6}	1.5×10^{-4}
WP108	9.9×10^{-6}	1.6×10^{-4}
WP109	8.8×10^{-6}	1.4×10^{-4}

14.5.7 Results: Farm Family Exposure at Tuff Site

GENII-S was used to analyze the pathway of the farm family exposed to usage of water from a well drilled at the site at 10,000 yr after closure. The exposure pathway includes drinking, irrigation, cattle and crop consumption using irrigation for feed and crops. The results of this calculation are given in Tables 14-24 and 14-25.

Table 14-24. Dose (rem) by Organ for Farm Family Exposure at Tuff Site

Organ	Mean	Max
Lung	1.1	16.0
Stomach	59.0	914.0
Small Intestine	2.1	32.0
UL Intestine	7.0	110
LL Intestine	19.0	296.0
Bone Surface	1.3	19.0
Red Marrow	1.3	19.0
Testes	1.1	17.0
Ovaries	1.1	17.0
Muscle	1.1	17.0
Thyroid	47.0	434.0
Kidneys	1.1×10^{-5}	30×10^{-4}
Liver	1.5	23.0
Spleen	2.8×10^{-11}	4.7×10^{-10}
Ingestion	11.0	162.0
Annual	11.2	162.0

Table 14-25. Dose (rem) by Radionuclide for Farm Family Exposure at Tuff Site

Radionuclide	Mean	Max
^{79}Se	1.5×10^{-11}	2.5×10^{-10}
^{99}Tc	10.6	162.0
^{129}I	0.56	9.9
^{234}U	4.1×10^{-6}	1.2×10^{-4}
^{236}U	2.0×10^{-9}	5.8×10^{-8}
^{235}U	2.4×10^{-12}	4.1×10^{-11}
^{231}Pa	1.5×10^{-7}	3.0×10^{-6}
^{237}Np	6.0×10^{-5}	1.0×10^{-3}
^{233}U	3.9×10^{-8}	1.4×10^{-6}
^{235}U	6.2×10^{-16}	1.8×10^{-4}
^{239}Pu	5.5×10^{-16}	7.7×10^{-15}

15. Performance Measures, Sensitivity Analysis, and Recommendations

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This chapter presents results from both the complex consequence models (Complex PA) and the simplified consequence models (Simple PA) in terms of the performance measures needed for comparison with the regulations, 40 CFR 191 and 10 CFR 60. This chapter begins with a description of these performance measures and an explanation of how the results are presented graphically (Section 15.1). Sections 15.2 and 15.3 discuss the comparison of the results with 40 CFR 191 for the Complex and Simple PAs, respectively, and Section 15.4 compares results between the Complex and Simple PAs. Section 15.5 discusses releases to the surface from cuttings/cavings, and Section 15.6 provides breach times and rates of release from the waste package. The parameters that influence the releases to the accessible environment are presented in Section 15.7. The chapter concludes with recommendations based on the findings from both the results presented in this chapter and the intermediate results found in the chapters on consequence models (Section 15.7).

15.1 Performance Metrics and Analysis Techniques

15.1.1 Performance Metrics

The relative ranking of the waste form depends upon the performance measures. For comparison with 40 CFR 191, the performance measure is the complementary cumulative distribution function (CCDF) of either EPA normalized releases or doses to individuals at the accessible environment over 10,000 yr (see Chapter 2). Because the radionuclide releases along the groundwater pathway are generally small, CCDFs at two other boundaries besides the disposal system boundary are used; these boundaries are at the water table directly below the repository and at the waste package (which includes the air gap around the waste containers). For comparison with 10 CFR 60, the performance measures are (1) the breach times of the waste parcels and (2) rates of release from the engineered barrier system (see Chapter 2).

15.1.2 Description of Terms and Graphic Presentation of Results

This section discusses the terms that are used to describe the results and explains how the results are presented graphically in this chapter.

Graphical Presentation of Results for 40 CFR 191. If the parameters ($\mathbf{x}$) of the consequence or probability model vary, the parameter variation (or uncertainty) is described mathematically as a cumulative distribution function (CDF) (or possibly as the derivative, or difference as appropriate, which is the probability density function [PDF]). When this parameter variation is propagated through the consequence model (C), the results, $C(\mathbf{x})$, will vary and the variation can be described again as a CDF, which plots the probability of a consequence occurring, $P(\mathbf{x}, S_j(\mathbf{x}))$, versus the consequence, $C(\mathbf{x}, S_j(\mathbf{x}))$. To make comparisons with the EPA limiting points specified in the Containment Requirements of 40 CFR 191, Section 13, or the Individual Protection Requirements of 40 CFR 191, Section 15, the CDF of the results is converted to a CCDF, where the CCDF is the "complement" of the CDF, or one minus the values of the CDF (1-CDF). (Throughout the remainder of this chapter, we have shortened "EPA limiting points specified in the Containment Requirements or Individual Protection Requirements of 40 CFR 191" to "EPA limiting line.")

Conditional CCDFs. When "conditional" CCDFs are presented in this report, the term "conditional" means that the CCDF is contingent on certain events or processes occurring. Most frequently, the selected event is a single intru-

sion into the repository (rather than many intrusions). Although multiple intrusions are a distinct possibility, the probability of their occurrence rapidly decreases as the number of intrusions increases. The construction of the conditional CCDF is performed with CCDFCALC in the CAMCON modeling system (see Figures 7-6 and G-1).

However, a clarification of the term "conditional" is necessary. Although CCDFs conditional on one selected event are presented, they actually are the mean of the CCDFs conditional on the one selected event *and* on the sampled parameters. The CCDFs that are conditional on both the selected event and sampled parameters are presented only once as a demonstration because a comparison with the EPA limiting line is inappropriate. (Note that in the latter case the number of CCDFs in the distribution is equal to the number of samples taken to propagate parameter uncertainty through the consequence or probability models; see Section 3.2.)

Composite CCDF. A composite, or complete, CCDF is also presented in this report.* The composite CCDF is the relevant measure of system performance for evaluating compliance with 40 CFR 191,[†] yet it subsumes so many events (such as multiple intrusions) that it is not often useful for understanding the behavior of a particular system component. Although the composite CCDF is the appropriate metric to compare with the EPA limiting line, no additional information from the consequence calculations is generated. Therefore, if an important goal of the analysis is understanding which parameters strongly influence the consequences, then using a CCDF conditional on one event, not a composite CCDF, is the more useful way to present these results.

Plotting CCDFs. A linear-arc hyperbolic sine plot, semilog plots, or the commonly used log-log plots are used for displaying composite and conditional CCDFs. To elaborate, because of the orders-of-magnitude change in consequences that make up the CCDF, the consequences are frequently displayed using a logarithmic scale on the abscissa. Here, however, the consequences (results from the consequence model) are sometimes shown on a similar arc hyperbolic sine scale ($\sinh^{-1}x = \ln(x + [x^2 + 1]^{1/2})$) since zero consequences can be plotted. Although not always the case for other PAs, the probabilities for this PA did not vary over orders or magnitude and so a linear scale was sometimes used on the ordinate of the CCDF graph. (Note, however, that the probability will necessarily not be one since the ordinate is $P[\hat{R} > R]$ not $P[\hat{R} \geq R]$.) A logarithmic scale for probability tended to obscure differences in the CCDFs at high probabilities and accentuated the differences at low probabilities.

Presenting the Contribution of Individual Radionuclides. The performance metric (R) for the Containment Requirements (Section 13) of 40 CFR 191 is the summed contribution from each radionuclide normalized by the corresponding EPA release limit (L_i) and waste unit factor (f_w) (see Chapters 2 and 3):

$$R = \frac{1}{f_w} \left(\frac{Q_1}{L_1} + \frac{Q_2}{L_2} + \dots + \frac{Q_i}{L_i} + \dots + \frac{Q_{nR}}{L_{nR}} \right)$$

where

$$Q_i = \text{activity released beyond a specified boundary } (q_i) \text{ integrated over } 10,000 \text{ yr} = \int_0^{10,000 \text{ yr}} q_i dt$$

Several times in this chapter, the distribution function of each normalized radionuclide ($Q_i/f_w L_i$) is presented rather than the sum (R). Furthermore, rather than presenting numerous CCDFs of ($Q_i/f_w L_i$), the PDFs are presented instead as "Tukey box plots," which are much easier to compare.[‡]

Variable Importance. The generation of scatterplots is the simplest sensitivity analysis technique and is sometimes used here to support a stated finding. This approach consists of generating plots of the results (dependent vari-

* A CCDF is generally described without the modifiers, "composite" or "complete", i.e., in most literature, a CCDF is referred to either simply as a CCDF (meaning a complete CCDF) or a conditional CCDF. However, in this chapter, we have chosen to modify a CCDF as "composite" when it is important to emphasize that a particular CCDF is not a CCDF conditional on one event.

[†] In actuality, the CCDF is still conditional because only exploratory drilling is assumed to occur and not, for example, purposeful intrusion. Nevertheless, the comparison with the EPA limiting line is appropriate because it also is conditional on only exploratory drilling occurring.

[‡] A box plot succinctly displays a PDF, e.g., the PDF of the results. See Chapter 8, where the PDF, CDF, and the box plot of the PDF, are presented for the model parameters that were varied in this report.

1 able value) vs. model parameters (independent variable value),** each point in the plot representing one "realization"
2 (deterministic calculation of probability and consequence models with one set of sampled model parameters). When
3 there is no relationship between the independent and dependent variable, the individual points are incoherently scat-
4 tered over the plot or spread along a horizontal line. In contrast, the existence of a well-defined relationship between
5 the independent and dependent variable is often revealed by patterns in the distribution of the individual points such
6 as a spread of points along a nonhorizontal locus.
7

8
9 **Graphical Results for 10 CFR 60.** The stochastic releases from the repository are compared with the regulatory
10 requirements on the waste package and engineered barrier specified in 10 CFR 60.
11

12
13 *Releases from Waste Package in First 300 Years.* 10 CFR 60 requires that "containment of HLW [high-level
14 waste] within the waste packages will be substantially complete" for at least 300 yr, where the waste package is the
15 waste parcel and any backfill or air gap directly around the waste parcel (see Chapter 2). At least three criteria can be
16 used to evaluate compliance with the requirement: (1) breach time of the last layer protecting the waste matrix,
17 (2) fraction of waste altered in first 300 yr, and (3) fraction of waste transported from the waste package in first
18 300 yr. All are useful and reported herein; however the latter criterion, fraction of waste transported from the waste
19 package, is used for comparison with the 10 CFR 60 requirement.
20
21

22
23 The presentation of the results is complicated, however, by the fact that different waste packages fail at different
24 times and under more than a single condition. For example, there is not single time when the disposal container or
25 last protective layer fails because the waste parcel consists of many layers and each waste type has different inner lay-
26 ers around the fuel or waste matrix. Also, each waste type represents a different proportion of the total inventory.
27 Finally, a distribution exists for breach times of layers, and fraction of waste altered or released, that depends on the
28 interplay of a variety of factors such as the location of the waste parcel in the repository and sampled corrosion rates.
29

30
31 In addition, the regulation does not specify whether limits for the 300-yr waste package requirement apply to
32 (a) statistical mean, median, or other quantile of the simulations run for compliance, (b) the worst of the simulation
33 set, or (c) a special simulation where all pertinent model parameters are set to either their most favorable, most unfav-
34 orable, median, or mean values. The approach here for issues (a) and (b) is to report the variation with time of the
35 sum of the fraction of each waste matrix exposed, altered, or transported, normalized by the EPA release limits. The
36 values are normalized so that the proportion of each waste type with important radionuclides is factored into the frac-
37 tion. The discussion in this chapter does not attempt to resolve issue (c); instead it presents without interpretation all
38 three types of comparisons. The reader is cautioned to note carefully the type of comparison being made.
39
40

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42 *Rates of Release from the Engineered Barrier.* 10 CFR 60 also requires that "the release rate of any radionuclides
43 from the engineered barrier system following the containment period shall not exceed one part in 100,000 per year of
44 the inventory of the radionuclides present at 1,000 yr ...," where the engineered barrier is the waste package and the
45 underground facility (underground structure, including openings and backfill materials). The same difficulties in pre-
46 senting the releases from the waste package described above apply to this measure as well, and the same approach to
47 resolving them was used here also.
48
49

50
51 Two additional difficulties occur for the rates of release. First, the magnitude of the release rate is dependent on
52 the time period, but the regulation is silent about the length of time over which the rate is to be evaluated. This time
53 period is significant with regard to how the simulations are run because time steps for the calculations must be on the
54 order of tens and sometimes hundreds of years to reasonably complete the stochastic analysis. Second, evaluating the
55 release rate from the *engineered barrier* is difficult. Omitting the underground structure potentially has a profound
56 influence on the reduction of release rates, as shown in the 1993 PA (Rechard, Ed., 1993), however measuring these
57 rates without including a small portion of the host rock is difficult because of the way in which the repository was
58 modeled in the 1994 PA. Consequently, to calculate release rates in the 1994 PA, the releases of any one radionuclide
59 from all waste packages are summed for each time step and then divided by the length of the time step.
60
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62
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64 ** The terms "dependent variable" and "independent variable" are used in the following paragraphs to emphasize that the result or model param-
65 eter may be modified to highlight relationships (e.g., the rank of a result may become the dependent variable and the rank of two or more model
66 parameters mathematically combined may become the independent variable).

15.1.3 Uncertainty Analysis Techniques

The purpose of uncertainty analysis is to determine the contribution (importance) of the uncertainty in the model parameters used in an analysis and the associated uncertainty in the result (usually consequences, $C[\mathbf{x}, S_j(\mathbf{x})]$, but sometimes probability, $P[\mathbf{x}, S_j(\mathbf{x})]$). Hence, "uncertainty" primarily means measures of the uncertainty in estimates for results of interest, including means, variances, and distribution functions. This section describes briefly the stepwise regression analysis technique used. A more detailed discussion of this technique and its application can be found in Helton et al., 1992; 1991.

In stepwise regression analysis, a sequence of regression models is constructed. The first regression model contains the single independent variable that has the largest impact on the dependent variable. The second regression model contains the two independent variables that have the largest impact on the dependent variable, the independent variable from the first step, plus whichever of the remaining variables has the largest impact on the variation not accounted for by the first step. Additional models are constructed in the same manner until a point is reached at which additional independent variables are unable to account meaningfully for the amount of variation in the dependent variable.

One way that the meaningful improvement is described mathematically is through the coefficient of determination r^2 . Further, the order in which the variables are selected in the stepwise procedure provides an indication of variable importance, with the most important variable usually being selected first, the next most important variable selected second, and so on. The r^2 values for each step in the regression analysis equal the fraction of the total variability in the dependent variable that can be accounted for by the individual independent variable added at that step. When the variation about the regression model locus is small, the corresponding r^2 value is close to 1, which indicates that the regression model is accounting for most of the variability in the dependent variable. Conversely, an r^2 value close to zero indicates that the regression model is not successful in accounting for the variability in the dependent variable. The absolute values of the standardized regression coefficients (SRCs) in the individual regression models also provide an indication of variable importance, and the sign of the SRC indicates whether the independent and dependent variables tend to increase and decrease together (a positive SRC) or tend to move in opposite directions (a negative SRC).

The statistical program, STEPWISE (Iman et al., 1980; Rechard, Ed., 1992, p. 12-13), was used to evaluate variable importance using the stepwise regression procedure on rank-transformed data. Regression analyses often perform poorly when the relationships between the independent and dependent variables are nonlinear. Poor linear fits to nonlinear data can often be avoided when the data are replaced with their corresponding ranks and the regression procedures are performed on these ranks (Iman and Conover, 1979).

It is necessary to have some criterion to stop the regression model construction process. In the analyses reported here, an alpha-value of 0.02 was used to add a variable to the regression model and a value of 0.05 to drop a variable from the model once added. (The alpha-value is the probability of obtaining a stronger relationship than the one identified in the analysis as a result of chance variation.) In addition, the Predicted Error Sum of Squares (PRESS) criterion (Iman et al., 1980) was used to protect against overfit.

As mentioned earlier in this report, sensitivity results are strongly dependent on the complexity of the models and the parameters that are *a priori* assumed to vary substantially. If modified conceptual models were used and other parameters were varied, the results might differ from those presented here.

15.2 Results from Complex PA

This section reports the individual doses and the summed normalized releases predicted by the consequence models for the Complex PA. The releases are shown for three locations. In general, the summed normalized releases are plotted with the corresponding probability of that release to form a CCDF. The individual doses are both plotted and tabulated. All figures for Section 15.2 can be found at the end of this section.

15.2.1 Individual Doses in First 10,000 yr at the Accessible Environment

Concentrations in the groundwater (pCi/liter) were examined at distances of 2.4 and 5 km from the repository. The concentrations at 2.4 km showed that the maximal dose over all sampled groundwater locations for all runs would have resulted in an individual whole-body dose of less than 1 μ Sv. (Most runs yielded much smaller doses.) The concentrations at 5 km were found to be even smaller than those at 2.4 km and were also small enough that they were within the range of numerical "noise" in the calculation of solute concentration in the transport simulations.

15.2.2 Release to Accessible Environment

Releases to the accessible environment from the tuff disposal system are presented in the form of composite CCDFs for both horizontal and vertical emplacement of the waste. The contribution of various radionuclides to this release is also discussed.

CCDF of Releases to Accessible Environment Assuming Horizontal Emplacement. The mean composite CCDF curve for horizontal emplacement when the waste is disposed of as a group lies to the left of the EPA limiting line, specified in the Containment Requirements of 40 CFR 191, Section 13, at all levels of probability for the tuff disposal system (Figure 15.2-1). This composite CCDF includes all releases (cuttings, liquid, and gaseous). As discussed later in Section 15.5, the direct releases from drill cuttings/cavings assume multiple intrusions within six intervals and a sampled drilling frequency for intruding into the repository in non-sedimentary rock of between 0 and 3 boreholes/km²/10,000 yr. These direct releases dominate the total releases below a probability of about 4%. When it is assumed that the entire contents of the MPC are brought to the surface, a few simulations intersect the EPA limiting line (Figure 15.2-1a). When a more realistic estimate is used, which assumes the contents from twice the diameter of the intrusion borehole are brought to the surface, no simulations intersect the EPA limiting line.

CCDF of Releases to Accessible Environment Assuming Vertical Emplacement. As with the CCDF for horizontal emplacement, the mean composite CCDF for vertical emplacement lies to the left of the EPA limiting line. Because the direct releases with vertical emplacement are much less than for horizontal emplacement, direct releases dominate only below a probability of about 0.1% (Figure 15.2-2).

The composite CCDFs of the releases at the surface from the gas movement up through the overlying strata and at a boundary 2.4 km laterally from the repository from groundwater transport are similar for both the horizontal and vertical emplacement schemes (Figure 15.2-3). The gaseous releases in the Complex PA for the mix of waste types are similar to the gaseous releases shown in the Simple PA for a repository filled with one spent fuel waste type (see Section 15.3).

Radionuclides Contributing to the CCDF for Horizontal and Vertical Emplacement. The list of important radionuclides changes depending upon where releases are monitored. The radionuclide contributing most to the total release to the accessible environment for both horizontal and vertical emplacement is ¹⁴C (Figure 15.2-4). The 99% or greater contribution swamps the contribution of most other radionuclides. In Figure 15.2-5, contribution of the radionuclides to groundwater release is shown for both the horizontal and vertical emplacement schemes. Roughly, the contribution for horizontal and vertical emplacement is ⁹⁹Tc, 82%; ¹²⁹I, 8%, ²³⁴U, 5%; and ²³⁷Np, 5%. This list of radionuclides differs substantially from the 1993 PA, primarily because retardation in the geologic barrier was neglected in the granite and salt disposal systems.

15.2.3 Individual Doses in First 10,000 yr at Various Points from Waterborne Sources

Figure 15.2-6 plots CCDFs for the Farm Well Pathway at 1000 m for the vertical and horizontal emplacement configurations at 10,000 yr. Figures 15.2-7 and 15.2-8 summarize dose by radionuclide and organ at 10,000 yr for both horizontal and vertical emplacement at the following two locations: intersection of well with the water table at (1) the downgradient edge of the repository and (2) 1000 m downgradient from the repository.

15.2.4 Individual Doses to 100,000 yr from Sources of Drinking Water

Figures 15.2-9 and 15.2-10 summarize dose by radionuclide and organ at 100,000 yr for both horizontal and vertical emplacement at the following locations: intersection of well with the water table at (1) the downgradient edge of the repository and (2) 1000 m downgradient from the repository. The doses were calculated using median model parameter values in a single deterministic calculation. Results from the analysis also predict that the organ with the relatively largest dose received is the bone surface.

For individual doses to 100,000 yr from sources of drinking water, ^{237}Np is the most important radioisotope considered because of its relatively long half-life (2.14 million yr), its relatively large internal dose conversion factor (3.9 for ^{237}Np compared to 1.3×10^{-3} for ^{99}Tc ; see U.S. DOE, 1988c), and its low retardation (see Chapter 5).

Figure 15.2-11 plots time histories of the contributions of ^{99}Tc and ^{237}Np to dose at 1000 m from the repository between 0 to 100,000 yr. Figure 15.2-11 also plots time histories of the contribution of ^{99}Tc to the doses (significant runs only) for the first 10,000 yr for the Farm Well Pathway (at 1000 m for both vertical and horizontal emplacement).

15.2.5 Release from Waste Package to Unsaturated and Saturated Zone

Results are presented in the form of mean conditional CCDFs for radionuclide activity released from the waste package to the unsaturated and saturated zones within the tuff disposal system for both horizontal and vertical emplacement of the waste.

Releases at Water Table Below Repository. The summed normalized releases from groundwater transport through the unsaturated zone to the water table below the repository (a monitoring point inside the tuff disposal system) are below the EPA limiting line for both the horizontal and vertical emplacement schemes in the Complex PA (Figure 15.2-12).

Releases from Waste Package. The normalized ^{14}C releases from the waste package to the unsaturated zone are below the EPA limiting line point while the liquid releases are not (Figure 15.2-13). This result is similar to the Simple PA.

Comparison of Figures 15.2-12 and 15.2-13 shows that while release from the waste emplacement packages is larger for the horizontal than for the vertical simulations, the reverse is true at the interface between the unsaturated and saturated zones. More of each radionuclide is released from the horizontally emplaced packages because more parcels breach; however, because the water flow rate is much lower, less of the radionuclide travels to the saturated zone.

15.2.6 Summary of Information Gathered about Total System Performance

Table 15.2-1 provides a summary of information gathered about the total system performance from the Complex PA.

Table 15.2-1. Summary of General Information Gathered on the Total Disposal System Performance

1. Mean individual doses from a farm family using well water from the aquifer underlying the repository at (a) the disposal system boundary (5 km from waste) and (b) 2.4 km from waste are too small to accurately calculate after 10,000 yr.
 - The CCDF of mean individual doses 1000 m from the waste before 10,000 yr is less than the EPA limit line of 150 μ Sv.
2. Individual doses at the disposal boundary (5 km from waste disposal region) for a farm family using well water from the underlying aquifer are very small.
 - Individual doses from the most important radionuclide, neptunium (^{237}Np)*, after 100,000 yr, at 1000 m from the waste, are 4.5 μ Sv for horizontal emplacement and 1 mSv for vertical emplacement; the doses were calculated using median parameter values.
 - Individual doses from neptunium at 1000 m from waste are 0.63 Sv when calculated using mean parameter values.
3. The complementary cumulative distribution function of EPA summed normalized releases indicates the examined waste form (Section ES.2.2), container (Section ES.2.3), repository layout (Section ES.2.4), and geologic barrier (Section ES.2.5) easily comply with the Containment Requirement of 40 CFR 191 (§13).
4. The radionuclides that contribute most to the EPA summed normalized release are as follows:* ^{14}C , ^{99}Tc , ^{129}I , ^{234}U , and ^{237}Np . (Because of the small inventory of ^{14}C for the DOE spent fuel and its total absence in the high-level waste, ^{14}C did not cause a violation of the Containment Requirement of 40 CFR 191.)
 - The determination of which radionuclides are important contributors is also sensitive to the regulatory period being considered, the performance metric (40 CFR 191 has been assumed here), and the location at which the metric is measured. This sensitivity and uncertainty regarding the form of the final regulations make it difficult, at this time, to identify radionuclides that should be immobilized or removed during treatment.

TRI-6342-5022-1

Figure 15.2-1. Composite complementary cumulative distribution functions (CCDFs) of total releases at the accessible environment (assuming 2.4-km boundary) for waste disposed of horizontally in rooms evaluated by the Complex PA consequence models. (a) Distribution of composite CCDFs for 36 simulations assuming contents of an entire MPC are brought to the surface during a human intrusion; (b) summary measures of the distribution of CCDF presented in figure a, including the mean, and 10%, 50% (median), and 90% quantiles; and (c) summary measures of distribution of composite CCDFs assuming the contents from twice the diameter of an intrusion borehole are brought to the surface cuttings/cavings.

TRI-6342-5023-1

Figure 15.2-2. Composite complementary cumulative distribution functions (CCDFs) of total releases evaluated at the accessible environment (assuming 2.4-km boundary) for waste disposed of vertically in boreholes for the Complex PA on log-hyperbolic sine axes. (a) Distribution of composite CCDF for 36 simulations, and (b) summary measures of the distribution of CCDF, including the mean, and 10%, 50% (median) and 90% quantiles.

TRI-6342-5024-1

Figure 15.2-3. Mean conditional complementary cumulative distribution functions (CCDFs) evaluated at the accessible environment for waste disposed of vertically and horizontally for the Complex PA on linear-hyperbolic sine axes. (a) Total releases (except cuttings) from the disposal system assuming a 2.4-km boundary, and (b) releases from the gaseous pathway and releases from groundwater pathway showing that gaseous releases dominate at high probabilities. (Cuttings dominate at low probabilities; see Section 15.5.)

15. Performance Measures, Sensitivity Analysis, and Recommendations

TRI-6342-5026-1

Figure 15.2-4. Contribution of 12 individual isotopes in Complex PA to summed normalized releases to the accessible environment (assuming 2.4-km boundary) for the tuff disposal system, assuming horizontal emplacement in disposal rooms (refer to Figure 15.2-3a). (a) Percentage of release and (b) summed normalized releases.

TRI-6342-5025-1

Figure 15.2-5. Contribution of 12 individual isotopes in Complex PA to summed normalized releases to the accessible environment from groundwater pathway. (a) Summed normalized releases for horizontal emplacement, (b) percentage of groundwater release for horizontal emplacement, (c) summed normalized releases for vertical emplacement, and (d) percentage of groundwater release for vertical emplacement.

TRI-6342-5101-0

Figure 15.2-6. Annual effective dose equivalent (E) for Farm Family Pathway for (a) horizontal emplacement and (b) vertical emplacement. In this pathway, it is assumed that a farmer drinks water from a well at the edge of the repository and 1000 m downgradient of the repository.

TRI-6342-5096-0

Figure 15.2-7. Dose in the water table at the downgradient edge of the repository for Farm Family Pathway at 10,000 yr for tuff repository for (a) radionuclide, horizontal emplacement, (b) radionuclide, vertical emplacement; (c) organ, horizontal emplacement, and (d) organ, vertical emplacement.

TRI-6342-5109-0

Figure 15.2-8. Dose at 1000 m for Farm Family Pathway at 10,000 yr for tuff repository for (a) radionuclide, horizontal emplacement, (b) radionuclide, vertical emplacement; (c) organ, horizontal emplacement, and (d) organ, vertical emplacement.

TRI-6342-5110-0

Figure 15.2-9. Dose in the water table at the downgradient edge of the repository for Farm Family Pathway at 100,000 yr for tuff repository for (a) radionuclide, horizontal emplacement, (b) radionuclide, vertical emplacement; (c) organ, horizontal emplacement, and (d) organ, vertical emplacement, using mean and median model parameter values.

(a) Horizontal Emplacement

(b) Vertical Emplacement

(c) Horizontal Emplacement

(d) Vertical Emplacement

TRI-6342-5111-0

Figure 15.2-10. Dose at 1000 m for Farm Family Pathway at 100,000 yr for tuff repository for (a) radionuclide, horizontal emplacement, (b) radionuclide, vertical emplacement; (c) organ, horizontal emplacement, and (d) organ, vertical emplacement.

TRI-6342-5102-0

Figure 15.2-11. Calculated doses of technetium-99 and neptunium-237 at well 1000 m downgradient of repository for (a) horizontal emplacement and (b) vertical emplacement. The doses were calculated from deterministic simulation using median model parameter values and show amounts of neptunium-237 increasing. The inlay shows doses from ^{99}Tc for the statistically significant runs from the total of 36 runs.

TRI-6342-5016-1

Figure 15.2-12. Mean conditional CCDF of radionuclide release at interface of unsaturated zone with saturated aquifer below the repository for both horizontal and vertical emplacement in the Complex PA. (a) Releases plotted on log-hyperbolic sine axes, and (b) releases plotted on linear-hyperbolic sine axes to show differences of horizontal and vertical emplacement at large probabilities.

TRI-6342-5029-1

Figure 15.2-13. Mean conditional CCDF of radionuclide releases from waste package of tuff disposal system for both horizontal and vertical emplacement evaluated by Complex PA consequence models. (a) Combined fluid (gas and liquid) releases showing overall releases are similar and (b) separate gas and liquid releases showing that releases for vertical emplacement are less than for horizontal emplacement at high probabilities but about the same for low probabilities.

15.3 Results from Simple PA

This section discusses the summed normalized releases predicted by the consequence models of the Simple PA, expressed as a CCDF. The releases are shown for three locations; all figures can be found at the end of this section.

15.3.1 Release to Accessible Environment

Releases to the accessible environment (5-km boundary^{††}) from the tuff disposal system are presented in the form of conditional CCDFs for both horizontal and vertical emplacement of the waste. Section 15.3.2 presents releases at two other locations within the tuff disposal system.

CCDF of Releases to Accessible Environment Assuming Horizontal Emplacement. The mean CCDFs of each waste type being placed in the repository fall into three groups (Figure 15.3-1):

1. The spent fuel waste parcels (Shippingport; ATR fuel; PWR fuel; and N-Reactor) have relatively high releases.
2. The high-level waste parcels from Savannah River, Hanford, and West Valley, have intermediate releases.
3. A spent fuel waste parcel (Fort St. Vrain) and the high-level waste parcels containing calcine from INEL — glass ceramic, borosilicate glass, and loose — have zero releases.

The zero releases for the parcel with Fort St. Vrain spent fuel and the high-level waste parcels containing calcine from INEL are explained easily since the temperature of the waste parcel remains below 60°C. At this temperature, corrosion of the Incoloy Alloy 825 is negligible. With no corrosion of the disposal container, no releases occur in 10,000 yr.

The spent fuel waste parcels with high releases are those dominated by ¹⁴C gas releases (Figure 15.3-1b). The ¹⁴C release dominates because of the much shorter gas transport time (less than 10,000 yr), relative to the aqueous transport, which takes more than 10,000 yr, even for the unretarded radionuclides. The waste parcels containing high-level waste in the intermediate and low release groups do not contain ¹⁴C, and thus have no gaseous releases.

Because the Incoloy Alloy 825 layer of the disposal container did not breach for the cool waste, several simulations were run without the Incoloy Alloy 825 layer (Figure 15.3-2). The low releases from the waste parcels containing the INEL calcine are caused by the small inventory of mobile aqueous species, such as ⁹⁹Tc and ¹²⁹I, and the absence of ¹⁴C. The waste parcels with INEL calcine do release some neptunium and other actinides in quantities similar to the other waste parcels, but the transport time of these radionuclides to the accessible environment is much greater than the time for ⁹⁹Tc or ¹²⁹I because of the retardation in the tuff.

To investigate the role of inventory in the relative releases from the waste parcels, we have calculated a “normalized inventory” (NI) which is given by

$$NI_{i,w} = I_{i,w} / (L_i fw_w)$$

where

$NI_{i,w}$	=	normalized inventory for isotope i and waste type w
$I_{i,w}$	=	initial inventory of isotope i in waste type w
L_i	=	release limit for isotope i per 1000 MTHM or other waste unit
fw_w	=	waste unit factor for waste type w

^{††} In the Simple PA, the saturated zone is modeled as a single porous medium without retardation for consistency with TSPA-1993 (Wilson et al., 1994); hence the saturated zone does not delay releases significantly and the 5-km boundary can be used in the Simple PA. In contrast, releases at the 5-km boundary are negligible in the Complex PA and so a 2.4-km boundary is used, as was used in the 1993 PA (see Section 15.2).

The normalized inventory is plotted in Figure 15.3-4.

For spent fuels, the releases to the accessible environment are dominated by the ^{14}C release to the surface so it is not surprising that the CCDF curves lie in the same order as the normalized ^{14}C inventory times the early clad failure fractions. $\text{NI} \cdot \text{ecff}$ is 1.9 , 2.0×10^1 , 6.0×10^{-2} , 5.7×10^{-2} , 4.1×10^{-3} for graphite, N-Reactor, Shippingport, PWR, and ATR fuels, respectively (Figures 15.3-1 and 15.3-1).

Because ^{239}Pu is very insoluble and highly retarded, it does not contribute to the liquid releases to the 5-km boundary. The summed normalized inventories excluding ^{239}Pu and ^{14}C multiplied by early clad failure fractions are 46, 45, 3, 0.7, and 0.2 for ATR, graphite, N-Reactor, Shippingport, and PWR fuels, respectively. This is the order of liquid releases seen at the 5-km boundary (Figures 15.3-1 and 15.3-1).

Note that the graphite fuel with a pre-breached Incoloy Alloy 825 layer in the disposal container has releases comparable to the N-Reactor fuel in the 1994 PA, while it was one of the best waste forms in the 1993 PA even without any container. This is due in part to the assumption made in the 1993 PA that all zircaloy clad would not be protective, thus increasing the releases from the PWR fuel by about two orders of magnitude in the 1993 PA. Also, ^{14}C was transported in the 1993 PA as dissolved CO_2 in the saturated repositories thus mitigating the graphite's very high ^{14}C inventory^{††}. Finally, in relation to the other fuels, the graphite fuel has the most unusual inventory of the waste types, with relatively high concentrations of ^{14}C , ^{231}Pa , ^{233}U , and ^{234}U , and very low concentrations of ^{238}U . Because the solubility of an isotope is dependent on its relative abundance, ^{234}U and ^{233}U have up to four orders of magnitude higher solubilities in the graphite fuel than the other fuels. Further, the graphite waste has relatively more parcels per unit of waste in the 1994 PA (Table 15.3-1) in order to "fill" a repository with one type of waste and yet have similar total heat and power outputs. The large number of waste parcels in turn increases the relative amount of advective and diffusive release for solubility-limited radionuclides, which is seen in the large contributions of ^{234}U and ^{233}U to the CCDFs of the graphite fuel.

Table 15.3-1. Number of Parcels Per Unit of Waste for Tuff Repository to Maintain Similar Total Heat Output and Power Density

Waste Parcel ID	Number of Waste Parcels Per Unit Waste	Waste Type	Heat Output (w)	Power Density (W/m^2)
101	2964	Fort St. Vrain	3.4323×10^6	3.7578
102	28	N-Reactor	3.4328×10^6	23.192
103	2327	Shippingport	3.4340×10^6	23.192
104	458	ATR	3.4354×10^6	23.192
105	222	PWR	3.4335×10^6	23.192
106	6365	Calcine in ceramic	3.4322×10^6	0.94274
107	164	Savannah River	3.4335×10^6	23.192
108	422	Hanford	3.4330×10^6	23.192
109	971	West Valley	3.4327×10^6	18.456
110	22,653	Calcine in glass	2.7761×10^6	0.25141
111	5428	Calcine, loose	3.4342×10^6	1.0703

For the high-level waste, the relative release is governed by the temperature of the repositories even when the Incoloy Alloy 825 layer of the disposal container is initially breached, because the carbon steel corrosion rate is also

^{††} Recall that ^{14}C is a concern only for the EPA summed normalized release and not for individual doses.

temperature dependent. The maximum waste parcel temperatures for Hanford, Savannah River, and calcine waste are 281°C, 124°C, and 32.2°C, which is reflected in the order of their releases (Figure 15.3-5). The three calcine waste types have similar maximum temperatures (31.5°C, 27.5°C, and 32.2°C) so their relative releases are determined by the matrix alteration rates, loose >> glass > glass-ceramic.

In summary, the factors that affect relative releases in Figures 15.3-1 through 15.3-3 include

1. Inventory — High relative inventory of the more mobile isotopes such as ^{14}C and the shorter-lived isotopes such as ^{234}U cause higher normalized releases.
2. Number of Disposal Containers Necessary to Accommodate Inventory — A large number of containers with small inventory will have relatively more advective and diffusive release of solubility-limited isotopes because of the larger collection area for water flow and possibility of more breach holes for diffusion.
3. Parcel Temperatures — Parcels that remain between 80°C and 100°C for long periods will have the greatest releases because more of the parcels within the repository will breach and because more temperature-dependent alteration of matrices such as UO_2 will occur. Parcels that are above 100°C will not breach until the temperature falls below 100°C, thus delaying the release of radionuclides. Delay in the release will substantially reduce the total release within 10,000 yr at the accessible environment.
4. Alteration Rate of Matrix — Fast-reacting matrices such as uranium metal, or uranium carbide, will release their soluble radionuclides very quickly, which will greatly increase their total releases.
5. Cladding — For corrosion-resistant cladding such as zircaloy and TRISO, the fraction that is damaged determines the fraction of the fuel that is exposed at early times.

The different behaviors of the groupings of CCDFs are also evident in the releases at monitoring points within the tuff disposal system, as discussed in the Section 15.3.2.

CCDF of Releases to Accessible Environment Assuming Vertical Emplacement. The mean CCDFs for the waste parcels, assuming vertical emplacement, are very similar to those assuming horizontal emplacement (Figure 15.3-3). The gas releases from the Shippingport and PWR spent fuels, however, are much lower in the vertical repository than in the horizontal repository. The only difference between the vertical and horizontal repository simulations that could affect the ^{14}C release is the waste parcel temperatures. In the horizontal emplacement simulations, the temperature of both these fuels rises above 100°C, while it does not in the vertical simulations. Because both the corrosion rate of the disposal container and the alteration rate of UO_2 matrix for the Shippingport and PWR spent fuel are temperature dependent, the rise above 100°C has a dramatic effect on the performance of these waste types. For the horizontal simulations (depicted in Figure 15.3-1b), one PWR and seven Shippingport simulations have no releases at all.*** In these simulations, no breaches occurred with the sampled corrosion rate of the Incoloy Alloy 825 layer of the disposal container and the repository temperature. As seen in Figure 15.3-3b for the vertical simulations, only 18 Shippingport and 14 PWR simulations have releases*, and the maximum releases have dropped from 4×10^{-2} to 8×10^{-3} , indicating that for those simulations for vertical emplacement with sampled corrosion rates high enough to readily breach, there are fewer locations in the repository with temperatures high enough to promote corrosion.

15.3.2 Release from Waste Package to Geologic Barrier

The radionuclides in the waste package leave either as gas and travel directly to the surface (accessible environment) or as dissolved species in water and travel down through the unsaturated zone and then laterally through the saturated zone to the tuff disposal system boundary 5 km from the repository. The gaseous releases (^{14}C) at the surface are only slightly reduced from those released at the waste package (Figure 15.3-5), whereas the aqueous releases are greatly reduced by passing through the geologic barrier. In general, only those dissolved radionuclides that are

*** The reader can attempt to verify this number by counting the steps in the mean conditional CCDF.

not retarded by the tuff, e.g., ^{99}Tc and ^{129}I , move through the geologic barrier. Therefore the calcine high-level waste, which has a lower recorded inventory of these two radionuclides, shows much lower releases than the high-level waste in borosilicate glass, regardless of the method of encapsulating the calcine (Figure 15.3-6). Because retardation was neglected in the 1993 PA for the salt and granite disposal systems, many radionuclides contributed to the releases, not just unretarded radionuclides. However, even when mobile radionuclides are present in the waste, e.g., in spent fuel, the geologic barrier is quite effective in reducing releases in 10,000 yr (Figure 15.3-7). In the consequence models for the Simple PA, the unsaturated zone represents the greatest barrier to release, whereas in the Complex PA the saturated zone is also a barrier. This difference occurs because the Simple PA assumes only a single porous medium without retardation in the saturated zone, consistent with TSPA-1993, whereas the Complex PA assumes a dual-porosity medium with some retardation, consistent with assumptions made by both the Simple and Complex PAs in the unsaturated zone.

15.3.3 Summary of Information Gathered about Waste Form

Table 15.3-2 provides a summary of information gathered about the waste form from the Simple PA.

Table 15.3-2. Summary of Information Gathered about Waste Form

-
1. Each waste form complies with Containment Requirements of 40 CFR 191 when placed individually in a repository; some even comply at the boundary of the waste parcel.
 2. Difference in performance of the waste types were due primarily to the temperature-sensitive corrosion rates and thus were influenced by differences in local temperatures around the container, which fluctuated because of substantial differences in heat output of the waste.
 - Other differences in waste types that affect performance include type and integrity of cladding, corrosion rate of waste form, and inventory (e.g., high-level waste does not contain ^{14}C).
 3. In general, high-level waste performs better than spent nuclear fuel.
 4. The Fort St. Vrain graphite fuel and INEL calcine high-level waste were too cool to obtain a 23.5 W/m^2 power density when placed individually in the repository (see Section ES.2.4, Repository Design); hence, the Incoloy Alloy 825 layer of the disposal container (see Section ES.2.3, Waste Container) did not fail for these waste types.
 5. For simulations where the Incoloy Alloy 825 layer is prebreached, the INEL calcine waste performs about the same as the DOE high-level waste within a repository as measured by the EPA summed normalized releases.
 - The rank order from best to worst is
 1. Calcine immobilized in glass-ceramic
 2. Calcine immobilized in borosilicate glass
 3. Savannah River sludge waste immobilized in borosilicate glass
 4. Hanford sludge waste immobilized in borosilicate glass
 5. West Valley sludge waste immobilized in borosilicate glass
 6. Calcine loose (similar to N-Reactor fuel and still within compliance; this latter option is not currently allowed because of prohibitions in 10 CFR 60 concerning particulates).
 - Calcine performs much better than the DOE glass in the geologic barrier because of the low inventory of technetium-99; this low inventory is possibly artificial and needs to be verified in future work.
 6. The performance of DOE spent fuels straddles the performance of pressurized water reactor (PWR) spent fuels when the measure is the EPA summed normalized release.
 - The rank order from best to worst is (order controlled by integrity or durability of cladding)
 1. Fort St. Vrain graphite fuels (uranium and thorium carbide with silicon carbide coating) (similar to N-Reactor fuel when there is no Incoloy Alloy 825 layer in disposal container)
 2. Shippingport (uranium dioxide fuel with zircaloy cladding)
 3. PWR (uranium dioxide fuel with zircaloy cladding)
 4. N-Reactor (uranium metal fuel with damaged zircaloy cladding)
 5. ATR fuel (uranium metal fuel with aluminum cladding)
 7. The heat of reaction of oxidizing all the uranium metal in N-Reactor fuel is about $1.34 \times 10^{13} \text{ J}$ or one-tenth of the heat energy produced in one year by radioactive decay of a 12,060-MTHM repository. Hence, while not small, the energy is not significant on a global scale in the 1994 PA calculation.
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(a) Liquid and Gas

(b) Gas

(c) Liquid

TRI-6342-5103-0

Figure 15.3-1. Mean conditional complementary cumulative distribution functions (CCDFs) for gaseous and groundwater releases only (no cuttings releases) at the 5-km boundary of accessible environment for waste disposed of horizontally in rooms evaluated by the Simple PA consequence models. (a) Combined gaseous and groundwater releases, (b) gaseous releases plotted separately showing that ^{14}C dominates releases from spent fuel (no ^{14}C exists in the high-level waste), and (c) liquid releases plotted separately.

(a) Liquid and Gas (No Incology)

(b) Gas (No Incology)

(c) Liquid (No Incology)

TRI-6342-5104-0

Figure 15.3-2. Mean complementary cumulative distribution functions (CCDFs) for gaseous and groundwater releases only (no cuttings releases) at the 5-km boundary to the accessible environment for waste disposed of horizontally in rooms evaluated by the Simple PA consequence models without an Incoloy Alloy 825 layer in the disposal container. (a) Combined gaseous and groundwater releases, (b) gaseous releases plotted separately, and (c) liquid releases plotted separately.

(a) Liquid and Gas

(b) Gas

(c) Liquid

TRI-6342-5105-0

Figure 15.3-3. Mean conditional complementary cumulative distribution functions (CCDFs) for gaseous and groundwater releases only (no cuttings releases) at the 5-km boundary to the accessible environment for waste disposed of vertically in boreholes evaluated by the Simple PA consequence models. (a) Combined gaseous and groundwater releases, (b) gaseous releases plotted separately showing that ^{14}C dominates releases from spent fuel (no ^{14}C exists in the high-level waste), and (c) liquid releases plotted separately.

(a)

(b)

TRI-6342-5129-0

Figure 15.3-4. Normalized inventory for the 12 isotopes selected for transport in the 9 waste types. (a) Spent fuels, and (b) high-level waste.

TRI-6342-5106-0

Figure 15.3-5. Comparison of gaseous releases from waste package and at surface, as computed by Simple PA. Plots show cumulative releases are reduced by only one-half order of magnitude by the geologic barrier.

TRI-6342-5107-0

Figure 15.3-6. Mean complementary cumulative distribution functions (CCDFs) for groundwater releases (gaseous releases are zero and cuttings releases are not included) from high-level waste as evaluated by Simple PA consequence models with no Incoloy Alloy 825 layer in disposal container. (a) Releases from waste parcel showing calcine in borosilicate glass or loose performs similarly to the borosilicate glass from Savannah River, Hanford, and West Valley, and (b) releases to the accessible environment showing calcine has zero releases to the accessible environment because of the low amounts of technetium-99 and iodine-129 currently reported for calcine.

(a) Fort St Vrain (No Inconel)

(b) Shippingport

(c) PWR

(d) N-Reactor

TRI-6342-5108-0

Figure 15.3-7. Mean conditional complementary cumulative distribution functions (CCDFs) for groundwater releases (gaseous releases and cuttings releases are not included) from spent nuclear fuel from waste parcel and to the accessible environment as evaluated by Simple PA consequence models. (a) Fort St. Vrain fuel (graphite) without an Incoloy Alloy 825 layer in disposal container, (b) Shippingport fuel (robust highly enriched fuel), (c) PWR fuel (low enriched fuel), and (d) N-Reactor fuel (weapons production fuel).

15.4 Comparison of Releases from Simple and Complex PAs

The conceptual models for the Simple and Complex consequence analyses are, in general, similar. The differences in the underlying conceptual models for the Simple and Complex PAs are highlighted below^{†††} followed by a brief discussion of the differences in releases.

15.4.1 Differences in Conceptual Models

A few major differences exist in the underlying conceptual models for the Simple and Complex consequence analyses (Table 15.4-1). The most apparent difference is in how the saturated zone aquifer was modeled. The Simple PA abstracted a velocity distribution and dispersivity from the TSPA-1993 (Wilson et al., 1994) that assumed only a single porous medium. These abstracted results were then used in a one-dimensional transport model without any retardation of contaminants. The Complex PA used fluid flow results directly in a corresponding transport model that included dual porosity and retardation of contaminants.

Several differences also exist between the two conceptual models in the modeling of the unsaturated zone, but the importance of these differences is not as readily apparent a priori. The differences include a one-dimensional versus two-dimensional model, single-phase versus two-phase flow, and uncoupling versus coupling of heat convection and transport (Table 15.4-1).

Table 15.4-1. Major Differences in Conceptual Models in Complex and Simple Consequence Analysis

Complex PA	Simple PA
Saturated Zone	
Dual porosity medium	Single porous medium
Retardation of radionuclides by sorption on tuff	No retardation of radionuclides
Three-dimensional model used directly in analysis	Abstraction of velocity distribution and dispersivity from three-dimensional model
Unsaturated Zone	
Liquid flow	
Two-phase flow	Single phase flow
Coupled heat convection and conduction	Uncoupled heat conduction
Two-dimensional model	One-dimensional model
Gaseous flow	
Identical to liquid flow	Abstraction of gas velocity from two-dimensional results reported in TSPA-1991 (Barnard et al., 1992)

15.4.2 Differences in the Results

The changes between the conceptual models for the Simple and Complex consequence analyses do produce noticeable differences in the EPA summed normalized releases, which appear in releases from the waste package even though the same source-term model was used (Figure 15.4-1a and b). These differences in results occur primarily because the current corrosion rates are very sensitive to temperature and differences exist between temperatures calculated for the area next to the disposal containers in the Simple and Complex PAs (Figure 15.4-2). Small differ-

^{†††} Although desirable, a verification of the Simple consequence analysis using an identical conceptual model for the Complex consequence analysis was not possible given the resource and time constraints of the 1994 PA study.

ences in the fluid flow from inclusion of two-phase flow and two-dimensional geometry within the geologic barrier account for the dramatically reduced release from the Complex PA, assuming horizontal emplacement (Figure 15.4-1c). The vertical emplacement did not have a similar effect since the initial saturation was set at 85% saturation rather than at 65% saturation, but the difference shows the importance of this parameter in the calculation. It also hints generally at the importance of initial conditions for the early times until assumed disruptive conditions overwhelm them at much later times (as shown in the discussion of the calculations out to 100,000 yr). The dramatic influence of a conceptual model that includes dual porosity and retardation is shown in Figure 15.4-1d, where liquid releases at the 2.4-km boundary are close to zero in the Complex PA but still noticeable in the Simple PA.

(a) Release of ^{14}C from Waste Package

(b) Liquid Release from Waste Package

(c) Liquid Release to Water Table

(d) Liquid Release to 2.4-km Boundary

TRI-6342-5112-0

Figure 15.4-1. Comparison of EPA summed normalized releases from Simple PA and Complex PA. (a) Release of carbon-14 from waste package showing that differences in releases exist at high probabilities but not at low probabilities, (b) liquid release from waste package, showing differences between the Complex and Simple PA, despite using the same source term, because temperatures are different, (c) liquid releases to water table showing that Complex PA with horizontal emplacement has smallest release to water table, and (d) liquid release to 2.4-km boundary, showing that Complex PA has negligible liquid release because of inclusion of retardation and dual permeability when modeling the aquifer.

TRI-6342-5065-

Figure 15.4-2. Comparison of temperatures calculated at wall of disposal container. (a) Complex PA with horizontal emplacement, (b) Simple PA with horizontal emplacement, (c) Complex PA with vertical emplacement, and (d) Simple PA with vertical emplacement.

15.5 Direct Release to Ground Surface During Drilling

The direct release of radionuclides to the accessible environment because of a drilling intrusion is based on the assumption that any hit on a waste parcel transports a large portion of the untransported contents of the waste parcel to the ground surface. That is, for this portion of the calculation it is assumed that all waste parcels are intact and that no radionuclides have leaked into the region surrounding the waste parcels. Thus, only waste parcel hits remove radionuclides. Figures depicting the results can be found at the end of this section.

15.5.1 Individual Doses from Exposure to Cuttings

Figure 15.5-1, which is a composite CCDF for all waste parcels, shows no violation of the EPA limit of 150 μ Sv for the annual effective dose equivalent. Shown are CCDFs for (a) vertical emplacement, (b) horizontal emplacement with the conservative assumption that an entire waste panel is removed upon interception by the drill, and (c) horizontal emplacement with the assumption that an area equal to twice the diameter of the intrusion borehole is removed. Refer to Section 15.5.2, "Cuttings Releases from Mixture of Waste Parcels," for a description of how probabilities of a drill bit hitting an individual waste parcel are calculated.

For individual dose, exposure to a driller occurs from only a single exploratory intrusion. The time, 7250 yr, was selected to demonstrate the results of this calculation. Other times were not examined for the tuff site.

Figure 15.5-2 summarizes the external dose for a driller when exposed to cuttings from each individual waste package.

15.5.2 Cuttings Releases from Mixture of Waste Parcels

The likelihood of the drillbit hitting a waste parcel during an intrusion is governed by a number of factors, including the number of waste parcel types within each group, the individual waste parcel cross-sectional area, the spacing of the waste parcels, and the drillbit area. Also considered in the final analysis is the probability that a drillbit will pass through the projected area of the repository. Assuming that the drillbit does hit the repository, the probability of a waste parcel hit was tabulated in Chapter 8 (Table 8-4) as a function of waste parcel number and waste emplacement orientation (horizontal or vertical).

Six times of intrusion were selected for consideration (125, 175, 350, 1000, 3000, and 7250 yr after emplacement). For comparison, the decay activity for the 22 waste parcels based on these six intrusion times is shown in Figures 9-1 through 9-23 (see also Appendix F). Figure 15.5-3 shows CCDFs that combine the probabilities and normalized releases for the waste in the tuff disposal system with horizontal and vertical emplacements. These types of plots, which total normalized releases, are used for comparison with the release limits specified in 40 CFR 191. Note, however, that the releases from fluid (gas and liquid) transport to the accessible environment are not included.

The cuttings release and the release due to groundwater flow and transport can be compared by overlaying Figures 15.5-3a and 15.5-3c on the figures for horizontal and vertical emplacements, Figures 15.2-1 and 15.2-2, respectively. For vertical emplacement, the smaller amount of radionuclides released from a hit generates cuttings/cavings releases with probabilities approximately one-tenth of those for the horizontal emplacement (compare Figures 15.5-3b and 15.5-3c). Consequently, the effect of cuttings on the CCDFs is considerably reduced, and cuttings releases from vertical emplacement do not approach the EPA limiting line.

15.5.3 Cuttings Releases from Individual Waste Parcels

The cuttings releases from one type of waste parcel placed in the repository show much less variation in the releases, than the ensemble. Furthermore, the resulting CCDFs are somewhat similar in shape with no violations of the EPA limiting line for both the horizontal (Figure 15.5-4) and vertical emplacements (Figure 15.5-5). The similarity in shape is because (1) factors influencing the probability axes of the CCDF such as frequency of drilling, the physical size of the waste containers, and the physical size of the repository, are the same for each waste type except for the Fort St. Vrain and calcine wastes, and (2) factors influencing the release axes while varying between them compensate for each other. Specifically, the amount of radionuclides released from an intrusion varies between the waste types as do the metric tons of heavy metal (MTHM) of the repository (the normalizing factor).

15.5.4 Summary of Information Gathered about Direct Releases

Table 15.5-1 provides a summary of information gathered about direct releases.

Table 15.5-1. Summary of General Information Gathered about Direct Releases

1.	Individual dose from one occurrence in the first 10,000 yr of a driller closely examining a 100-mm-dia sample from an MPC for one hour, and with continued incidental exposure to cuttings from the entire MPC for one week thereafter ("groundshine"), is no more than 3 μ Sv.
2.	For horizontal in-drift emplacement in an MPC, the probability of direct cuttings release is about eight times greater than for vertical emplacement in boreholes; direct cuttings release is also about eight times greater for horizontal emplacement than for vertical (assuming entire contents of container is brought to surface in each case).

TRI-6342-5121-0

Figure 15.5-1. External dose from geologist closely examining a small amount of cuttings/cavings 7250 yr after emplacement for one hour and groundshine for one week from exposure to cuttings from the contents of twice the diameter of the intrusion borehole, an entire MPC, and an entire LWT for horizontal and vertical emplacement, given the probability of hitting various types of waste.

TRI-6342-5122-0

Figure 15.5-2. External dose from geologist examining cuttings/cavings 7250 yr after emplacement for each type of waste parcel for (a) horizontal and (b) vertical emplacements.

(a) Entire MPC

(b) Portion of MPC

(c) Entire LWT

TRI-6342-5027-1

Figure 15.5-3. Composite CCDF of summed normalized releases from cuttings/cavings from the tuff disposal system ($\lambda^* = 3$ borehole/km²/10,000 yr) for mixture of all waste types for (a) horizontal emplacement assuming contents of an entire MPC brought to surface, (b) horizontal emplacement assuming contents from twice the diameter of the intrusion borehole from an MPC are brought to surface, and (c) vertical emplacement assuming entire LWT brought to surface.

TRI-6342-5037-1

Figure 15.5-4. Composite CCDF of summed normalized releases from cuttings/cavings from the tuff disposal system ($\lambda^* = 3$ borehole/km²/10,000 yr) containing individual waste types placed horizontally in rooms of the repository. (a) spent fuel waste parcels and (b) high-level waste parcels.

TRI-6342-5038-1

Figure 15.5-5. Composite mean CCDF of summed normalized releases from cuttings/cavings from the tuff disposal system ($\lambda^* = 3$ borehole/km²/10,000 yr) containing individual waste types placed vertically in boreholes of the repository. (a) spent fuel waste parcels and (b) high-level waste parcels.

15.6 Release from the Waste Package (Complex PA)

In general, release of radionuclides from the waste parcels can be thought of as occurring in three steps:

- (1) **Breach.** Breach of all containment layers.
- (2) **Alteration.** Alteration of matrix materials, thus liberating radionuclides.
- (3) **Release.** Transport from the parcel through the air gap and/or rubble to the host rock.

If any of these three steps can be delayed, then release from the waste parcel is greatly delayed. 10 CFR 60 specifies that the waste package must provide "substantially complete containment for 300 to 1000 years" and also specifies the maximum allowable release rate per year for each radionuclide from the engineered barrier. In addition, 40 CFR 191 specifies the allowable cumulative release to the accessible environment and individual doses in 10,000 yr. The amount and timing of radionuclide release from the waste parcel have a direct effect on the amount of release at the accessible environment. This section describes these three steps and compares the results to the regulations.

15.6.1 Breach Times

The penetration of a waste parcel is dependent upon a number of factors including:

- Type of waste parcel layers.
- Corrosion rate of parcel layers; both generalized and localized corrosion.
- The moisture near the parcel layers.
- The temperature of the parcel layer.

Depending on the values of parameters sampled in this performance assessment, a range of breach times is observed for the waste parcels. "Breach time" or "exposure time" is defined for each matrix within a waste parcel as the time when the last layer protecting the matrix is breached and the matrix is exposed to groundwater. The size of the breach may range from a pinhole to the entire surface area of the layer. A breach time is associated with each matrix of each waste parcel within each container group and repository grid block (see Chapter 11 for discussion of container groups). In addition, for waste parcels with fuel cladding that has failed before disposal ("early clad failure fractions"), there is an exposure time for the spent fuel with initially failed cladding and a later breach time for the spent fuel with initially intact cladding. Consequently, there are 2204 breach times for the horizontal emplacement repository and 1444 breach times for the vertical emplacement repository. The results are grouped and summarized here.

To measure how effectively the engineered barrier system prevents the waste from contact with groundwater, the FWE, the fraction of waste exposed to groundwater, has been defined. When only one type of waste is emplaced in the repository, FWE is easy to calculate. However, when various types of spent fuel are mixed with high-level waste, a weighting factor is needed for each waste type. For this calculation, the waste unit factor (f_w) (see Section 15.1.2) is defined as the weighting factor in 40 CFR 191. At each time step, the source term submodel, USATCONC, checks the breach state of all layers of each waste parcel in each container group in each grid block. When USATCONC detects that the breach of a layer exposes a matrix, it calculates the fraction of the repository waste that is contained within that matrix and adds that fraction to the total FWE.

Figures 15.6-1a and 15.6-1b show the FWEs over the 10,000-yr regulatory period for the 36 simulations in the Complex PA for the tuff disposal system for horizontal and vertical emplacements, respectively. The mean and various quantiles calculated from the 36 simulations are also shown. A wide range of waste parcel behavior is depicted, with many simulations showing a significant portion of the waste eventually exposed. Figures 15.6-2a and 15.6-2b show these same results for the first 300 yr only. Figures 15.6-1c through 15.6-1f and 15.6-2b show the fraction of waste that is altered and released and are included here so they can be easily compared to the fraction of waste exposed, but their results will be discussed in Sections 15.6.2 and 15.6.3.

To better understand Figure 15.6-1, we must look more closely at the breach times for individual waste packages and the parameters that affect them. Figure 15.6-3 shows the minimum, average, and maximum breach times for each waste package and container group for horizontal emplacement, using median values for all parameters. The container groups (CGs) used in the 1994 PA were defined based on the initial integrity of the carbon steel overpack and the integrity of the air gap, as shown in Table 15.6-1. The minimum, average, and maximum breach times for each waste package have been presented to show the variation that occurs due to the temperature and water saturation differences across the repository. Three main features of the proposed waste emplacement packages affect the parcel breach times: the air gap, the cladding, and the temperature of the wall of the disposal container.

Table 15.6-1. Container Groups

Container Group	Good Overpack	Good Air Gap	Fraction of Waste Parcels in Simulation with Median Parameter Values
1	yes	yes	0.4975
2	no	yes	0.0025
3	yes	no	0.4975
4	no	no	0.0025

The Effect of the Air Gap. As seen in Figure 15.6-3, the container groups with a good air gap (Container Groups 1 and 2) show much less corrosion and thus much later breach times than the container groups with an air gap that has been bridged by rubble (Container Groups 3 and 4). The difference results from the method used to model contact of the waste parcels with water, using the saturation-dependent corrosion term in the source term submodel (see Chapter 11).

To elaborate, the source term submodel, USATCONC, assumes that a threshold fracture saturation exists below which wet corrosion will not occur unless the air gap is bridged. In the 1994 PA, the threshold saturation for waste parcels with intact air gaps was assumed to be the residual saturation of the fracture (4%), while the threshold saturation for waste parcels with rubble was assumed to be 0%. The 4% threshold was chosen for the waste parcels with an air gap because the only methods in which the waste parcels could become wet are condensation, dripping, and flooding. Condensation was considered unlikely, and neither dripping nor flooding was expected to occur with fracture saturations below residual.

With a collapsed tunnel or collapse of the structure supporting the container, matrix flow could also provide a means of bringing water into contact with the waste parcel. At early times, before a significant amount of corrosion products have formed on the parcel, it would be difficult for the matrix water to overcome capillary forces to leave the matrix and flow onto the waste parcel, but at later times the corrosion products would remove that capillary barrier, so a threshold of 0% fracture saturation for waste parcels with a bridged air gap was chosen. As discussed in Chapter 12, calculated fracture saturations are mostly clustered between 2% and 3.5% (see Figures 12-10e and 12-10f). Some simulations show an increase above residual after 2,000 yr, but the simulation using median values for all the parameters does not go above residual until about 9,000 yr. From Chapter 11 (Figure 11-2), it can be seen that this range of fracture saturations results in a saturation term of 0.68 to 0.87 for the waste parcels with rubble, and 0.0 for waste parcels with an intact air gap. These saturation terms result in the use of the much faster wet corrosion rate for waste parcels with rubble and the much slower humid corrosion rate for the waste parcels with an intact air gap, which is reflected in the early breach times for Container Groups 3 and 4 in Figure 15.6-3.

The Effect of the Clad. The effect of cladding can be seen in the breach times for waste parcels with graphite, N-Reactor, Shippingport, and PWR spent fuels (WPs 101,102,103 and 105). For each of these waste parcels, two groups of breach times are shown (Figure 15.6-3): the first for the exposure time of the matrix within fuel rods with initially damaged cladding and the second for the matrix within fuel rods with initially intact cladding. The fraction

that is damaged (the early clad failure fraction for each waste parcel) is given in Table 15.6-2, which also lists the waste type, waste unit factor, and protective layers for each waste parcel. The TRISO cladding of the Fort St. Vrain fuel particles (WP101) was assumed to be very corrosion resistant, which is reflected in the bars that show no exposure for Fort St. Vrain with intact clad at any location within the repository and in any container group. The corrosion rate for zircaloy, which was determined by experiment, is quite slow and is reflected in its earliest breach at 12,675 yr.

Table 15.6-2. Parameters for Waste Parcels in Complex PA

Waste Parcel ID	Waste Type	Waste Unit Factor	Protective Layers*	Early Clad Failure Fraction (Median Value)
101	Graphite (Fort St. Vrain)	0.028	Carbon steel, Incoloy Alloy 825, TRISO coating	0.045
102	Weapon fuel (N-Reactor)	2.10	Carbon steel, Incoloy Alloy 825, Zircaloy clad	0.33
103	Robust highly enriched spent fuel (Shippingport)	0.110	Carbon steel, Incoloy Alloy 825, Zircaloy clad	0.01
104	Highly enriched spent fuel (ATR)	0.072	Carbon steel, Incoloy Alloy 825, Aluminum clad	0
105	Low enriched spent fuel (PWR)	0.162	Carbon steel, Incoloy Alloy 825, Zircaloy clad	0.01
106	Calcine high-level waste (INEL glass-ceramic)	0.32	Carbon steel, Incoloy Alloy 825	0
107	High-level waste (Savannah River borosilicate glass)	8.04	Carbon steel, Incoloy Alloy 825	0
108	High-level waste (Hanford borosilicate glass)	1.16	Carbon steel, Incoloy Alloy 825	0
109	High-level waste (West Valley borosilicate glass)	0.071	Carbon steel, Incoloy Alloy 825	0

* Stainless steel layers were assumed to crack and thus afford no protection.

The Effect of Temperature. The effect of temperature can be seen by the variation of breach times for each waste parcel. Figure 15.6-5 shows the breach times across the repository from the center at block 1 to the edge at block 29 for waste parcels with the hottest temperature (ATR fuel, WP104), the coolest (calcine in glass-ceramic, WP106), and intermediate (N-Reactor, WP102). (See Figure 12-23 for the waste parcel temperatures at the center of the repository). In Figure 15.6-5a, ATR fuel (WP104) shows late breach times because it is above the boiling point longer than any other waste parcel. As the repository cools, the ATR fuel waste parcels at the edge of the repository drop below the boiling point first and thus breach first. Figure 15.6-6a shows the temperature profile across the repository for ATR fuel waste parcels at four times. The difference in the breach times for Container Groups 3 and 4 show that for ATR fuel, the carbon steel overpack offers additional protection between 100 and 250 yr.

In Figure 15.6-5c, calcine in glass-ceramic (WP106) shows some of the earliest breach times; however, in six grid blocks, it never breaches. As seen in Figure 15.6-6b (see also Figure 12-23), the temperature of this waste parcel never rises above boiling and thus the waste parcel starts to undergo wet corrosion immediately. With an activation energy term of 2530 K (21 kJ/mole), the generalized corrosion rate of carbon steel is only moderately temperature dependent, but with an activation energy term of 19,600 K (162 kJ/mole), the localized pit corrosion of Incoloy Alloy

825 is highly temperature dependent. At 100°C, a wet Incoloy Alloy 825 layer will breach in about 20 yr; at other temperatures, the time for breach is as follows: 90°C, 85 yr; 80°C, 394 yr; 70°C, 2000 yr; and 60°C, 11,000 yr. Figure 15.6-6b shows that when calcine waste parcel (WP106) is at the center of the repository, it takes about 80 yr to drop from 93°C to 89°C. Not surprisingly, Figure 15.6-5c shows that calcine in glass ceramic (WP106) in Container Group 4 lasts 85 yr at the center of the repository. It is not surprising that at the edge of the repository, where the initial temperature of calcine in glass ceramic is about 70°C, dropping below 60°C by 100 yr, calcine waste parcels in Container Group 4 do not breach. It is interesting to note the difference in behavior of calcine in Container Groups 3 and 4 at grid block 23. Without the protection of the carbon steel overpack, calcine in Container Group 4 breaches in 348 yr, but with the protection of the overpack during the crucial warm years, calcine in Container Group 3 never breaches.

Figure 15.6-5b shows features similar to both 15.6-5a and 15.6-5c. The N-Reactor waste parcel (WP102) is initially above boiling except at the edges of the repository. As it cools, the first grid block to breach is block 21. This grid block is the first one to stay in the crucial temperature range of 80°C to 100°C long enough for the Incoloy Alloy 825 layer to breach. Blocks closer to the edge of the repository drop below 80°C too quickly and thus take longer to breach, while the block closer to the center stays above 100°C longer and thus delays the start of wet corrosion.

Reviewing all the waste parcels in Figure 15.6-3a, it can be seen that all waste types have some parcels that have not been breached by 100,000 yr with the exception of the hottest waste types, ATR (WP104) and Hanford (WP108). Like calcine (WP106) and N-Reactor (WP102), the edge of the repository cools too quickly for the Incoloy Alloy 825 to breach in these waste parcels. The coolest waste packages have the earliest breaches: 60 yr, for graphite (WP101); 85 yr, for calcine (WP106). The hottest waste packages have the latest first breaches: 1235 yr, Hanford; 1394 yr, ATR. The rest of the waste parcels have first breaches in the range of 139 to 158 yr. The ATR waste parcel is also interesting because it is the only waste parcel to show breaches in the container groups with an intact air gap (Figure 15.6-7). Wet corrosion cannot occur in Container Groups 1 and 2 until the fracture saturation rises above residual and dripping occurs. In the simulation with median parameter values, this occurs at about 9000 yr when the ATR waste parcels in the center of the repository are about 65°C. At 65°C, it takes about 5500 yr to breach 2 cm of wet Incoloy. Because the temperature is slowly dropping at 9000 yr, it takes even longer and the first breach is seen at 15,500 yr (Figure 15.6-7). The fall in the temperature of several degrees for the waste parcels toward the edge of the repository at these late times causes a dramatic increase in the breach times.

While each breach shown in Figures 15.6-3b through 15.6-3e are reflected in the FWE curve of 15.6-3a, some waste parcels types contain more waste (as measured by the waste unit factor for each waste parcel type) and thus have more effect on the FWE curve. While breaches of waste parcels for N-Reactor, Shippingport, PWR, Savannah River, and West Valley contribute to the early rise in the fraction of waste exposed between 200 and 500 yr, only the rise as the result of breaches from waste parcels for N-Reactor and Savannah River is noticeable. The fraction of waste in Savannah River (WP107, in Container Groups 3 and 4) is 0.3345, the fraction of waste in N-Reactor (WP102, with damaged clad in Container Groups 3 and 4) is 0.029, and the fraction of West Valley (WP109, in Container Groups 3 and 4) is 0.003. Similarly, the rise in the FWE curve at 2000 yr includes contributions from ATR and Hanford (WP104 and WP108, in Container Groups 3 and 4), which have waste fractions of 0.003 and 0.048 respectively. The large rise at 20,000 yr in the FWE curve is due to the breach of the initially undamaged zircaloy clads in N-Reactor (WP102, in Container Groups 3 and 4) (a waste fraction of 0.058).

Returning to Figure 15.6-1a, it appears that the air gap effectively protects the waste parcels during the first 10,000 yr. Therefore, the maximum fraction of the repository waste that may be exposed is given by the fraction of waste parcels that has a bridged air gap ("BACFR" in Chapter 11, Table 11-7). Because this parameter was sampled with a uniform distribution between 0 and 1, the FWE curves at 10,000 yr would be uniformly distributed between 0 and 1 if all waste parcels with rubble breached. For the simulation using the median values of all the parameters, the waste parcels with undamaged zircaloy, undamaged TRISO, and the waste parcels at the edge of the repository did not breach by 10,000 yr, thus the FWE was 0.355, or 0.145 lower than the fraction of waste with rubble. Because the corrosion rates of carbon steel, Incoloy, and zircaloy were sampled, as well as the flow and climate parameters that affect the fracture saturation, the fraction of waste that remains unbreached within Container Groups 3 and 4 will vary with each simulation. The relatively uniform distribution of FWE curves at 10,000 yr between 0 and 0.75, however, is an indication of the good correlation between the fraction of waste exposed and fraction of waste parcels with a

bridged air gap (BACFRC). Figure 15.6-1b shows the FWE curves for the vertically emplaced waste parcels. In these simulations, there are far more waste parcels that never breach (seen in the larger average breach times in Figure 15.6-3b), due to the lower temperatures of these waste parcels. Figures 15.6-8a and 15.6-8b show the breach times for Hanford waste parcels (WP107 and WP207) for the simulations using median values for all parameters. WP207, Container Group 4, shows earlier breach times than WP107, Container Group 4, but there are also nearly 0.2 of WP207, Container Group 4, that never breach while 0.1 of WP207, Container Group 4, never breach. WP207, Container Group 3, shows later breaches than WP107, Container Group 3, and there are nearly 0.5 of WP207, Container Group 3, that never breach while 0.2 of WP207, Container Group 3, never breach. Similarly, for N-Reactor, ATR, PWR, and West Valley waste parcels (WPs 202, 204, 205, and 209, Container Group 4), the vertical simulations show earlier breach times than the horizontal, but there are also more waste parcels that never breach in the vertical simulations than the horizontal.

15.6.2 Alteration of Matrices

Once a matrix is exposed to groundwater after breach of the overlying protective layers, the portion of the radionuclides that have migrated to readily accessible locations, such as the gap between the fuel matrix and cladding or grain boundaries within the fuel matrix, are released, but the remaining radionuclides are "bound" within the matrix. Alteration of the matrix starts immediately, and proceeds at the sampled alteration rate. As the matrix is altered, radionuclides are uncovered, but insoluble elements such as Pu dissolve only up to their solubility limit. ^{14}C is assumed to be released into the gaseous phase as CO_2 once it is released from alteration of the matrix, and highly soluble elements such as iodine are expected to dissolve completely in the pore fluids. Thus while breach times discussed in the previous section determine what fraction of the waste is exposed to groundwater, the alteration rates determine the rate at which the radionuclides are released from the matrices.

Figures 15.6-1c and 15.6-1d show the fraction of waste altered in the horizontal and vertical emplacement simulations. In both cases the fraction of waste altered is significantly smaller than the fraction of waste exposed. This difference is due to the slow alteration rate of the borosilicate glasses, and the disproportionate fraction of the waste that is in the Savannah River waste parcel (WP107). In the few simulations where large glass alteration rates were sampled, the fraction of waste altered makes a steady climb until all the exposed glass is altered, at which time the fraction of waste altered levels out. Figure 15.6-2c shows a close-up of the fraction of waste altered in 300 yr in the horizontal emplacement simulations.

While the calculated median value from these 36 simulations in 300 yr is 9% for the fraction of waste exposed, it is only 0.6% for the fraction of waste altered. The plots of fraction of waste exposed, "FWE curves," of the vertical emplacement simulations start climbing sooner than the horizontal emplacement simulations but reach smaller values at 300 yr. This difference is because boiling at the waste parcel wall delays wet corrosion for the hotter horizontal repository. The cooler vertical repository has earlier breach times because many parcels do not go over the boiling point, but it also has more parcels that never breach because they are too cool. The delay is more pronounced in the plots of fraction of waste altered, "FWA curves," because the matrix alteration routines use the higher waste parcel centerline temperature in determining whether the matrix is wet or above boiling, and it takes longer for the waste package centerline to drop below boiling than the outer wall of the waste parcel. This longer delay causes the FWA curves for the horizontal emplacement to remain below those of the vertical simulations over the 300 yr.

15.6.3 Release from the Waste Package

Fraction of Waste Released. Once released from the matrix, radionuclides may precipitate and remain within the waste parcel, or they may dissolve in groundwater and be released from the waste package by advection and/or diffusion. In addition, radioactive decay and in-growth will affect the amount of each radionuclide moving from one

location to another. Figures 15.6-1e and 15.6-1f show the fraction of waste that is released (FWR)^{†††} from the waste package across the air gap or rubble. Figures 15.6-9a and 15.6-9b show the FWR curves in log space, and Figures 15.6-2e and 15.6-2f show close-ups of the first 300 yr. The dramatic reduction from the fraction of waste altered to fraction of waste released seen in Figures 15.6-1 and 15.6-2 is due to the very slow rate of diffusion across the rubble and very slow water flow rate through the repository. As described in Chapter 11, the relative importance of the advective and diffusive release within these calculations is dependent on the flow rate within the fractures and matrices, the effective collection area of the waste parcels, and the effective diffusion area term. The flow rate provided by the two-phase modeling code, BRAGFLO_T, is dependent on all of the sampled flow and climate parameters such as permeability and infiltration amplitude. However, the effective collection area of the waste parcels and the effective diffusion area terms are sampled parameters directly used by the source term submodel, USATCONC.

10 CFR 60 requires "substantially complete containment" of the radionuclides within the engineered barrier system during the first 300 yr. The medians of the FWR curves for the horizontal and vertical emplacement simulations at 300 yr are 2×10^{-5} and 4×10^{-5} respectively, and the maximums are 6×10^{-4} and 3×10^{-3} . It is not clear whether these fractions of waste released meet the definition of "substantially complete containment."

In Figures 15.6-1, 15.6-2, and 15.6-9, the early releases from the repository with vertically emplaced waste are higher than those from the repository with horizontally emplaced waste while the opposite is true at later times. The maximum fraction of waste released in 10,000 yr is 2.4×10^{-1} for both the vertical and horizontal emplacement simulations but the median fraction of waste released is 1.4×10^{-3} and 3.2×10^{-4} for the horizontal and vertical simulations, respectively.

The advective and diffusive releases from a single simulation of each repository can be seen in Figure 15.6-10a, which shows the cumulative curies of ^{237}Np released by advection and diffusion in the simulations using median values for all parameters. At early times, when the fracture saturation is below residual, there is very little flow of fluids through the parcels so the release is dominated by diffusion. The vertical emplacement simulation shows earlier diffusive releases because there are earlier breaches; it shows earlier advective release because there is more downward flow through the vertical repository due to higher initial TCw saturations (see Chapter 12). After 10,000 yr, there are more advective releases than diffusive releases, and the horizontal emplacement simulation has more advective releases than the vertical emplacement simulation. The factors that affect the relative releases due to advection and diffusion in the two repositories include the fraction of waste altered, the effective collection areas for water flow into the parcels, the effective areas for diffusion from the parcels, and the flow of water through the repository.

The fraction of waste altered is larger after 300 yr in the horizontal simulation using median values for all the parameters, which leads to larger releases from the horizontal simulation at later times as seen in Figure 15.6-10a. Larger releases from the vertical simulation occur at early times. In addition, the total collection area for advection is $31,277 \text{ m}^2$ in the horizontal emplacement repository and $10,062 \text{ m}^2$ in the vertical emplacement repository, so this term is three times larger for horizontal emplacement than for vertical emplacement. The total surface area of the parcels is $116,703 \text{ m}^2$ and $197,318 \text{ m}^2$ for horizontal and vertical emplacements, respectively; the air gap is 0.1 m and 0.025 m for horizontal and vertical emplacements, respectively. These differences result in a diffusive area/diffusive length term that is nearly eight times larger in the vertical emplacement repository than in the horizontal emplacement repository. These two effects tend to make diffusion relatively more important in the vertical emplacement repository, as seen in Figure 15.6-10a.

^{†††} To calculate the fraction of waste released, we used the following formula:

$$FWR = \sum_i \frac{R_i}{L_i} / \sum_i \frac{I_i}{L_i}$$

where

FWR = fraction of waste released,

R_i = curies of released radionuclide i ,

L_i = 40 CFR 191 release limit in curies per unit waste for radionuclide i ,

I_i = the initial inventory of radionuclide i in curies.

i = the 12 isotopes chosen for modeling by the transport code.

Note that ^{239}Pu has 99% of the summed normalized initial activity of these 12 isotopes.

The only other effect that makes a large difference in the behavior between the two orientations is the water flow rates. Early time flow rates are affected by the initial saturation of the tuff, while late time flow rates are affected by the increased percolation of water through the tuff from climate changes. As discussed in Chapter 12, the vertical simulation used an initial saturation of 0.85, which resulted in more downward flow through the repository for vertical emplacement. Figure 15.6-11 shows the vertical flow rate of water through the bottom of the repository in the simulation using the median values for all parameters. Notice that the scale of the vertical emplacement simulation plot is three orders of magnitude larger than the horizontal emplacement plot. The climate model uses an infiltration frequency of 80,000 yr for the simulation with median values, which results in a maximum infiltration at 40,000 yr. In the simulation with median values, it takes about 10,000 yr for the change in infiltration at the surface to reach the repository, so the maximum flow occurs around 50,000 yr. In this simulation, the percolating water flow first becomes significant at 9000 yr when the matrix saturation goes to 1 and the fracture saturation rises above residual (see Chapter 12, Figure 12-10). This is reflected in Figure 15.6-10a by the rapid rise in the advection releases at about 9000 yr and a tapering off of the advective releases after 50,000 yr. The larger flow of water in the vertical simulation causes larger advective releases from the vertical simulation at early times, as can be seen in Figures 15.6-1, 15.6-2, 15.6-9, and 15.6-10a.

Figure 15.6-12c shows the fraction of the release of ^{237}Np that is due to diffusion in the 36 simulations of the horizontal emplacement repository, and Figure 15.6-12b shows the mean, 10%, 50%, and 90% calculated from the 36 simulations. In each simulation, the fraction of release is undefined before the first release. For nearly all simulations, the fraction of release due to diffusion jumps to about 1.0 at the time of breach and then decreases. The amount of decrease and the time of decrease are different for each of the simulations. The mean of the 36 simulations has an initial peak of about 0.8 at 900 yr indicating that at 900 yr about 20% of the vectors have not yet breached. Two sampled parameters have a direct effect on the relative importance of advection versus diffusion, the effective collection area, and the effective area for diffusion. The effective collection area was assigned a loguniform distribution from between one-half order of magnitude smaller than the cross section of the parcel to one-half order of magnitude larger than the cross section of the parcel. This distribution results in an order of magnitude range in the advective releases when all other factors are kept constant. The effective area for diffusion (Chapter 11) captures the uncertainty in the size of the breach (from a pinhole to the size of the entire surface area of the parcel) and the tortuosity of the diffusive pathway. Because a 1-mm pinhole is over six orders of magnitude smaller than the surface area of the parcel and the tortuosity of unsaturated gravels can easily exceed 10^4 , the loguniform distribution ranging from 10^{-6} to 1 is expected to be conservative. The six-order-of-magnitude range in the diffusive releases is responsible for most of the wide range of fractions of release.

Release Rates - Simulation using Median Values for All Parameters. Besides the 300-yr requirement on the waste parcel, 10 CFR 60 has a release rate limit for individual radionuclide release from the engineered barrier system (see Chapter 2 and Appendix C). The distributions of release rates for several radionuclides are presented in this section for comparison with the release rate requirements of 10 CFR 60.

Figure 15.6-13a shows the normalized release rate of six radionuclides from the horizontal emplacement simulation using median values for all the parameters. The release rate from this single simulation is shown because when individual runs are averaged, an artificial smoothing of the curves results. Also, the simulation using median values was run past 10,000 yr, where much of the interesting behavior is seen.

The release rate curves in Figure 15.6-13 show two basic shapes. The very soluble elements such as C, Tc, and I, show very spiky release rates because of the rapid release that occurs from the quick release of radionuclides in grain boundaries in UO_2 fuels (PWR and Shippingport) and fast alteration of UC_2 , UAl_x , and U metal fuels (Fort St. Vrain, ATR, and N-Reactor). Because these elements are very soluble, rapid release may occur even when water flow is very small. The more insoluble elements such as U, Np, and Pu, show much smoother release rate curves that are more closely correlated with the total amount of water flowing through the containers.

The first feature of the ^{99}Tc release rate curve (Figure 15.6-13a) is a sudden rise in release rates around 60 yr followed by a drop off. This rise is due to the breach of the coolest waste parcels: Fort St. Vrain (WP101, Container Groups 3 and 4) and the calcine in glass-ceramic (WP106, Container Group 4). These waste parcels first breach in the hot portion of the repository at 60 and 85 yr, respectively, and then gradually breach toward the cooler edges of the repository (Figure 15.6-4c). The sudden rise in the ^{99}Tc release rate followed by a drop is due to the Fort St. Vrain

waste parcel (WP101, Container Group 3) breaching in 16 blocks at 76 yr, 3 blocks at 79 yr, and only one block at a time after that. The Fort St. Vrain waste parcel, WP101, is expected to be more important than the calcine in glass-ceramic because the UC_2 matrix alters in about 17 yr, while the glass-ceramic alters very slowly. Because ^{99}Tc is highly soluble, the matrix alteration rate controls its release rate. The similarity in shape between the ^{99}Tc and ^{14}C curves confirms this expectation because the calcine waste does not contain ^{14}C . Note that the relative importance of the waste parcels for the release rate curves is different from the relative importance of the waste parcels for the fraction of waste exposed (FWE) and fraction of waste altered (FWA). For the release rate, the alteration rate of the waste parcel matrices is more important, while for the fraction of waste exposed (FWE) and fraction of waste altered (FWA), the waste unit factor is more important.

The next feature of Figure 15.6-13a is the ^{99}Tc peak starting at 200 yr and continuing to 400 yr. In this time period waste parcels for N-Reactor, Shippingport, PWR, Savannah River, and Hanford (WPs 102, 103, 105, 107 and 109) all have breaches in both Container Groups 3 and 4. Waste parcels for Shippingport, PWR, Savannah River, and Hanford raise the ^{99}Tc release rate baseline to about 0.068 of the allowable release rate because of the slow release from UO_2 and glass. However, the quick release of ^{99}Tc from grain boundaries in the Shippingport and PWR waste parcels and the release from the reactive U metal within the N-Reactor waste parcel are responsible for the peak of over 2.5 times the allowable release rate. Figure 15.6-5b shows the corresponding breach times ranging from 200 to 400 yr for N-Reactor waste parcel (WP102), Container Groups 3 and 4, with defective zircaloy clad.

The third feature in the release rate of ^{99}Tc in Figure 15.6-11a is the peak between 1400 and 2800 yr. During this period only the two hottest waste parcels, ATR and West Valley, are breaching. While breach of the West Valley waste parcel (WP108) raises the baseline ^{99}Tc release rate to 0.133 of the allowable release rate, the fast reacting UAl_x fuel in the ATR waste parcel (WP104) raises the peak to above 3.6. During this period, all of the ATR fuel with rubble breaches (Figure 15.6-5a).

At 12,000 yr, the originally intact zircaloy claddings of Container Groups 3 and 4 of the Shippingport and PWR waste parcels start to fail. The especially large peak at 13,600 yr is due to the quick release fraction from Shippingport (WP103, Container Group 3, in blocks 5 to 22). At this point in the calculation the time steps average about 250 yr. If the calculation used 1-yr increments instead, this peak could potentially be two orders of magnitude larger. (On the other hand, use of the mean of the 36 simulations, or other statistical measure of the distribution, greatly smooths the peaks.) Between 15,500 and 18,000 yr, the only waste parcels to fail contain the ATR fuel and have intact air gaps (WP104, Container Groups 1 and 2, Figure 15.6-7). Only the hottest waste parcels remain intact long enough to experience significant corrosion at later times when a wetter climate causes fracture flow and dripping onto the containers. All of the ATR waste parcels (WP104) breach within 100,000 yr, but only the Hanford waste parcels (WP108) in the center two grid blocks breach. The peaks after 15,500 yr are shorter than the one at 13,600 yr because they are caused by breaches of WP104 in only one grid block at a time. After 18,000 yr, the peaks get even shorter because the time steps go from 250 to 1000 yr. The peaks between 18,000 and 54,000 yr are due to breach of zircaloy in N-Reactor waste parcels (WP102) and continued breach of ATR fuel waste parcels (WP104) with an intact air gap. With no additional breaches after 54,000 yr, the release rate remains steady around 0.119 of the allowable release rate until 97,000 yr when it drops dramatically to 0.005 at 100,000. While part of the decline of the ^{99}Tc release rate at 97,000 yr is due to its half-life of 213,000 yr, most of it is the result of the depletion of an altering matrix, since the same behavior is seen in ^{129}I (a drop of 1.3 orders of magnitude from 4.8×10^{-6} to 2.1×10^{-7}). Figure 15.6-2a shows that the fraction of waste altered quickly approaches the fraction of waste exposed at 100,000 yr, and so only a small portion of the breached containers have unaltered waste by 100,000 yr.

The curves for ^{99}Tc , ^{14}C and ^{129}I are similar because none of their releases is solubility limited. Carbon-14, however, shows decay after 1000 yr due to its 5730-yr half-life and its release rate peaks occur one time step ahead of ^{129}I and ^{99}Tc because it is released as a gas during the time step of breach instead of in the liquid during the next time step. The individual release limits for ^{99}Tc , ^{14}C , and ^{129}I are 0.512, 0.0036, and 0.00029, respectively, but the alternate release rate limit, 0.018, was used for ^{14}C and ^{129}I . The use of the alternate release rate limit (see Chapter 2 and 10 CFR 60.113 in Appendix C) versus the individual release rate limit accounts for some of the offset between the normalized curves for these isotopes.

The curves for ^{235}U , ^{237}Np , and ^{239}Pu are quite different due to their much lower solubility as well as radioactive in-growth. The rise and fall of ^{237}Np between 100 and 400 yr is due in part to the decay of its parent ^{241}Am (half-life,

432 yr). It is also possible at these early times that the amount of ^{237}Np liberated from the matrices is low enough that its solubility limit has not been reached and thus its release rate is correlated with the alteration of the N-reactor fuel. The rise in the release rates around 13,000 yr is due in part to the increase in the number of waste parcels containing enough altered matrix to satisfy the solubility limit. The more containers that are at the solubility limit, the more release there can be from diffusion and advection. This rise, however, is also due to the increased water flow through the repository caused by the climate model. As previously described, the flow rate increases steadily until the time of maximum infiltration at 50,000 yr. The first significant flow occurs when the tuff matrix becomes fully water saturated and the saturation of the fracture rises above residual saturation at around 9000 yr; the maximum flow through the repository occurs around 50,000 yr. This is reflected in a rise in the release rate starting at 9000 yr and a maximum in the release rates for the solubility limited elements at around 50,000 yr. Because the ^{239}Pu curve parallels the longer lived ^{235}U and ^{237}Np curves, it is clear that decay does not deplete ^{239}Pu enough to affect the release rate.

Release Rates - 36 Simulations.

Carbon-14. ^{14}C is the primary radionuclide influencing the total cumulative releases from the spent nuclear fuel (see Figure 15.2-4, Section 15.2.1). The mean and median of the distribution of release rates for ^{14}C exceeds the total release rate limit for all radionuclides of 0.018 Ci/yr in 10 CFR 60 but does not exceed the EPA Containment Requirements. Both the release rate of each sample set and the summary statistics of the release rates are shown in Figure 15.6-14.

Technetium-99. ^{99}Tc is an important contributor to radionuclide releases from the groundwater pathway (see Section 15.2.1). The mean and median of the distribution of release rates for ^{99}Tc exceeds the allowable release rate of 0.5 Ci/yr (see Chapter 4 for allowable release rates for individual radionuclides) (Figure 15.6-15a).

Iodine-129. ^{129}I is also an important contributor to radionuclide release from the groundwater pathway (see Figure 15.2-4, Section 15.2.1), but does not exceed the total release rate limit for all radionuclides of 0.018 Ci/yr (Figure 15.6-15b).

Uranium-235. Although the release rate of ^{235}U exceeds its allowable release rate in two simulations (Figure 15.6-16a), it is below 0.1% of the total release rate limit of 0.018 Ci/yr for all radionuclides (the alternative criterion - see Chapter 2), and thus complies with 10 CFR 60. However, ^{235}U is an important radionuclide for criticality calculations (see Chapter 10).

Neptunium-237. ^{237}Np is another important contributor to radionuclide release from the groundwater pathway, but does not exceed the total release rate for all radionuclides of 0.018 Ci/yr (Figure 15.6-16b).

Plutonium-239. For aqueous releases, ^{239}Pu is an important contributing radionuclide (see Section 15.2.1) (Figure 15.6-17). The distributions of the release rates from the horizontally and vertically oriented waste parcels are similar and both comply with the 10 CFR 60 release limits.

15.6.4 Summary of Information Gathered about the Waste Containers

Table 15.6-3 summarizes the information gathered about the waste containers.

Table 15.6-3. Summary of Information Gathered about the Waste Containers

1. Based on current literature values for corrosion rates of carbon steel and Incoloy Alloy 825 at temperatures near 100°C with oxygen and water, many of the disposal containers breach rapidly. However, breaching of the disposal containers does not necessarily imply complete release of radionuclides because other protective layers must also be breached, the matrix containing the radionuclides must be altered, and the radionuclides must be transported out of the parcel. Three fractions of waste have been calculated for comparison with the 10 CFR 60 waste package requirement: the fraction of waste exposed, the fraction of waste altered, and the fraction of waste released.

	After 300 yr			
	horizontal emplacement		vertical emplacement	
	median*	maximum	median	maximum
fraction of waste exposed	9×10^{-2}	6×10^{-1}	3×10^{-2}	6×10^{-1}
fraction of waste altered	6×10^{-3}	7×10^{-2}	6×10^{-3}	7×10^{-2}
fraction of waste released	2×10^{-5}	6×10^{-4}	4×10^{-5}	6×10^{-3}

- The fraction of waste altered is significantly lower than the fraction of waste exposed due to the slow alteration rates of the glass and UO_2 matrices. Jumps in the fraction altered are due to fast reacting matrices such as the ATR and N-Reactor fuels.
 - The fraction of waste released is significantly lower than the fraction altered because of the slow flow of water through the parcels and slow diffusion of radionuclides through breaches in the parcels.
 - Because the pitting rate of Incoloy Alloy 825 is reported to be highly temperature dependent in the literature**, the parcel temperatures dominate the breach times of the parcels that have contact with water.
 - The dependence of the corrosion rates on fracture saturation implemented in the source term submodel, USATCONC, results in very little corrosion of parcels with intact air gaps.
2. Several of the radionuclide release rates exceed the allowable rate from the engineered barrier specified in 10 CFR 60. Both the mean and median release rates of ^{99}Tc and ^{14}C exceed the allowable release rate.
3. The retardation of radionuclides by sorption onto rust particles (assuming adequate oxygen) only somewhat reduced releases of liquid-transported radionuclides to the host rock.
4. The high-level waste performs well enough that a robust disposal container is not needed except for compliance with arbitrary requirements in 10 CFR 60.

* The NRC does not state in 10 CFR 60 precisely what "substantially complete" means in quantitative terms nor what probability should be used to compare release rates.

** The reader should consult Chapter 11 for a full description of the temperature-dependent rates.

TRI-6342-5099-0

Figure 15.6-1. *Fraction of waste, over the 10,000-yr regulatory period for the 36 simulations for the tuff disposal system. (a) Exposed to groundwater, horizontal emplacement, (b) exposed to groundwater, vertical emplacement, (c) altered, horizontal emplacement, (d) altered, vertical emplacement, (e) released from waste emplacement package, horizontal emplacement, and (f) released from waste emplacement package, vertical emplacement. The mean and various quantiles calculated from the distribution of 36 simulations are also shown.*

(a) Horizontal

(b) Vertical

(c) Horizontal

(d) Vertical

(e) Horizontal

(f) Vertical

TRI-6342-5100-0

Figure 15.6-2. Fraction of waste, over the 300-yr period for the 36 simulations for the tuff disposal system. (a) Exposed to groundwater, horizontal emplacement, (b) exposed to groundwater, vertical emplacement, (c) altered, horizontal emplacement, (d) altered, vertical emplacement, (e) released from waste emplacement package, horizontal emplacement, and (f) released from waste emplacement package, vertical emplacement.

TRI-6342-5035-1

Figure 15.6-3. The minimum, average, and maximum breach times for each waste emplacement package and container group for the simulations of the tuff repository with horizontal emplacement, using median values for all model parameters. (a) Fraction of waste exposed and altered versus time, (b) Container Group 1 (good carbon steel, good air gap), (c) Container Group 2 (initially failed carbon steel, good air gap), (d) Container Group 3 (good carbon steel, bridged air gap), and (e) Container Group 4 (initially failed carbon steel, bridged air gap).

TRI-6342-5038-1

Figure 15.6-4. The minimum, average, and maximum breach times for each waste emplacement package and container group for the simulations of the tuff repository with vertical emplacement, using median values for all model parameters. (a) Fraction of waste exposed and altered versus time, (b) Container Group 1 (good carbon steel, good air gap), (c) Container Group 2 (initially failed carbon steel, good air gap), (d) Container Group 3 (good carbon steel, bridged air gap), and (e) Container Group 4 (initially failed carbon steel, bridged air gap).

(a) ATR

(b) N-Reactor

(c) Calcine in Ceramic

TRI-6342-5115-0

Figure 15.6-5. Breach times across the horizontal repository of Container Groups 3 and 4 using median values for all parameters. (a) ATR fuel (WP104), (b) N-Reactor fuel (WP102), and (c) calcine in glass-ceramic (WP106).

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TRI-6342-5116-0

Figure 15.6-6. Temperatures of the outer walls of waste parcels across the horizontal repository using median values for all parameters. (a) ATR fuel (WP104) and (b) calcine in glass-ceramic (WP106).

TRI-6342-5117-0

Figure 15.6-7. Breach times across the horizontal repository using median values for all parameters for Container Groups 1 and 2, ATR fuel (WP104).

TRI-6342-5124-0

Figure 15.6-8. Breach times across the repository for Savannah River glass using median values for all parameters. (a) Horizontal emplacement (WP107) and (b) vertical emplacement (WP207).

TRI-6342-5118-0

Figure 15.6-9. Fraction of waste release from the waste parcels. (a) Horizontal emplacement and (b) vertical emplacement.

TRI-6342-5098-0

Figure 15.6-10. Releases of ^{237}Np from the simulations using median values for model parameters. (a) Cumulative releases (curies) from diffusion, advection, and ingrowth, in the vertical and horizontal repositories, and (b) fraction of release due to diffusion.

TRI-6342-5119-0

Figure 15.6-11. Water flow rate (matrix and fracture) through the bottom of the repository grid blocks using the median parameters. (a) Horizontal emplacement, initial saturation, 0.65, and (b) vertical emplacement, initial saturation, 0.85.

TRI-6342-5123-0

Figure 15.6-12. Fraction of release of ^{237}Np due to diffusion in the horizontal simulations. (a) Fraction of release for 36 simulations and (b) summary statistics calculated from the 36 simulations.

(a) Horizontal Emplacement

(b) Vertical Emplacement

TRI-6342-5120-0

Figure 15.6-13. Selected radionuclide release rates normalized by the allowable release rates according to 10 CFR 60 using median parameter values. (a) Horizontal emplacement and (b) vertical emplacement.

(a) ^{14}C Sample Sets (b) ^{14}C Summary

TRI-6342-5125-0

Figure 15.6-14. Distribution of release rates of ^{14}C evaluated by Complex PA consequence models from the horizontal waste emplacement package. (a) Release rate of each sample set and (b) summary statistics of release rates, including mean, and 10%, 50%, and 90% quantiles.

(a) ^{99}Tc

(b) ^{129}I

TRI-6342-5126-0

Figure 15.6-15. Distribution of release rates of radionuclides evaluated by Complex PA consequence models from the horizontal waste emplacement packages for comparison with 10 CFR 60. Quantiles of (a) ^{99}Tc and (b) ^{129}I .

TRI-6342-5127-0

Figure 15.6-16. Distribution of release rates of radionuclides evaluated by Complex PA consequence models from the horizontal waste emplacement packages for comparison with 10 CFR 60. Quantiles of (a) ^{235}U and (b) ^{237}Np .

(a) ^{239}Pu Horizontal Emplacement (b) ^{239}Pu Vertical Emplacement

TRI-6342-5128-0

Figure 15.6-17. Distribution (quantiles) of release rates of ^{239}Pu evaluated by Complex PA consequence models from the waste emplacement packages. Rates show the similarity in overall distributions of release rates between the horizontally and vertically oriented waste emplacement packages. (a) Waste emplaced horizontally in rooms and (b) waste emplaced vertically in boreholes.

15.7 Important Parameters Influencing the Releases

15.7.1 Important Parameters in Simple PA

Twenty-two cases including the five spent fuel and six high-level waste cases for both horizontal and vertical orientations were analyzed with STEPWISE: WP101 through WP111 for the horizontal orientation and WP201 through WP211 for the vertical orientation. The strongest correlations between the dependent parameter, EPA summed normalized release of radionuclides, and the independent parameters sampled were the global parameters related to climatic cycle period and infiltration during a climatic cycle. This statement holds true for both horizontal and vertical waste emplacement groups. These sampled parameters influenced the flow of water through the tuff disposal system. While a few of the sampled parameters influenced transport of radionuclides through the tuff disposal system, none showed a strong correlation with total release. The only other sampled parameter that showed marked correlation with total summed normalized release was the Incoloy Alloy 825 corrosion rate for both horizontal and vertical emplacement cases.

15.7.2 Important Parameters for Complex PA

For the Complex PA, sampled parameters were evaluated against releases of individual radionuclide species for three separate cases:

- Liquid and gaseous releases from the waste parcels
- Liquid and gaseous releases from the repository
- Liquid releases to the water table.

In general, correlations between sampled parameters related to fluid flow ("flow" parameters) and radionuclide releases were dominated by climatic variables, especially for liquid releases to the water table for both horizontal and vertical emplacement. Climatic variables were less dominant at the repository boundary and from the waste parcels themselves, because other sampled parameters exerted their influence over releases. For vertical emplacement, the corrosion rate of Incoloy Alloy 825 correlated strongly with both liquid and gaseous releases. For horizontal emplacement, the climatic variables, especially the climatic cycle period, remained as the most important. In both cases, other sampled parameters showed correlation with releases for individual radionuclides but to a lesser extent than those just mentioned. For example, for the sampled parameters related to contaminant transport ("transport parameters"), the effective area for diffusion from the disposal container proved to be highly correlated with liquid radionuclide release for most of the radionuclides tracked (see discussion in Section 15.6). This correlation was true for releases from the waste parcels and at the repository boundary for both horizontal and vertical emplacement. However, liquid releases to the water table did not correlate strongly with this or any other parameter.

In addition, regression analysis was completed for the flow sample with respect to repository water and gas flow rates. For both horizontal and vertical emplacement, these flow rates were dominated by the sampled climatic parameters, with the climate cycle period showing the greatest correlations with the flow rates, followed by the base infiltration rate and the infiltration amplitude.

15.7.3 Summary of Influential Parameters

Tables 15.7-1 and 15.7-2 list the sample parameters influencing groundwater and gaseous releases for the Simple PA for horizontal and vertical emplacement, respectively. Table 15.7-3 lists the sample parameters influencing groundwater and gaseous releases for the Complex PA.

Figures 15.7-1 and 15.7-2 show scatterplots of the more influential parameters in the Simple and Complex PAs, respectively.

Table 15.7-1. Sampled Parameters Influencing Groundwater and Gaseous Releases from Tuff Disposal System in the Simple PA for Horizontal Orientation

Waste ID	Description	Minimum infiltration	Return period of climate change	Maximum infiltration	Corrosion rate of Incoloy Alloy 825	Fraction of disposal containers contacting rubble	Plutonium absorption coefficient on rust of container
101	Graphite (Fort St. Vrain)	--	--	--	--	--	--
102	Weapon fuel (N-Reactor)	0.54*, 0.29**	-0.54, 0.24	0.36, 0.13	0.42, 0.20	--	--
103	Robust HEU (Shippingport)	0.36, 0.14	--	--	0.52, 0.28	--	0.40, 0.19
104	HEU (ATR)	0.55, 0.24	0.53, 0.29	0.36, 0.13	0.59, 0.33	--	--
105	LEU (PWR)	0.56, 0.27	-0.37, 0.13	0.31, 0.09	0.65, 0.42	0.32, 0.09	--
106	Calcine HLW, INEL, glass ceramic	--	--	--	--	--	--
107	HLW, Savannah River, borosilicate glass	--	--	--	0.83, 0.69	--	0.40, 0.16
108	HLW, Hanford, borosilicate glass	0.49, 0.24	-0.53, 0.23	--	--	--	--
109	HLW, West Valley, borosilicate glass	--	--	--	--	--	--
110	HLW, INEL, calcine, borosilicate glass	--	--	--	--	--	--
111	HLW, INEL, calcine, loose	--	--	--	--	--	--

* Standardized regression coefficient (SRC) of regression model
 ** Coefficient of determination (r^2)

Table 15.7-2. Sampled Parameters Influencing Groundwater and Gaseous Releases from Tuff Disposal System in the Simple PA for Vertical Orientation

Waste ID	Description	Minimum infiltration	Return period of climate change	Maximum infiltration	Corrosion rate of Incoloy Alloy 825	Fraction of disposal containers contacting rubble	Plutonium adsorption coefficient on rust of container	Technetium fraction released immediately for matrix 2
201	Graphite (Fort St. Vrain)	--	--	--	--	--	--	--
202	Weapon fuel (N-Reactor)	0.52*, 0.22**	-0.47, 0.23	0.37, 0.14	0.65, 0.40	0.30, 0.09	--	--
203	Robust HEU (Shippingport)	0.26, 0.07	--	--	0.77, 0.64	--	0.37, 0.14	0.45, 0.17
204	HEU (ATR)	0.52, 0.27	-0.54, 0.25	0.37, 0.13	0.72, 0.51	0.25, 0.07	0.33, 0.11	0.48, 0.22
205	LEU (PWR)	--	--	--	0.80, 0.64	--	0.43, 0.16	0.38, 0.15
206	Calcine HLW, INEL, glass ceramic	--	--	--	--	--	--	--
207	HLW, Savanna River, borosilicate glass	--	--	--	0.80, 0.65	--	0.43, 0.16	0.41, 0.17
208	HLW, Hanford, borosilicate glass	0.48, 0.23	0.48, 0.20	0.32, 0.10	--	--	--	--
209	HLW, West Valley, borosilicate glass	0.49, 0.24	-0.49, 0.21	0.32, 0.10	--	--	--	--
210	HLW, INEL, calcine, borosilicate glass	--	--	--	--	--	--	--
211	HLW, INEL, calcine, loose	--	--	--	--	--	--	--

* Standardized regression coefficient (SRC) of regression model
 ** Coefficient of determination (r^2)

Table 15.7-3. Sampled Parameters Influencing Groundwater and Gaseous Releases from the Tuff Disposal System in the Complex PA for Horizontal and Vertical Orientations

Waste Container Orientation	Fraction of containers contacting rubble	Corrosion rate of Inconel	Transport dispersivity fraction	Uranium solubility in silica-saturated water	Return period of climate change	Saturated hydraulic conductivity of matrix in TSW layer
Release from Waste Parcels						
Horizontal						
¹²⁹ I	0.77*, 0.60**	--	--	--	--	--
²³⁹ Pu	--	--	-0.26, 0.06	--	--	-0.43, 0.18
²³⁸ U	--	--	--	--	--	--
Vertical						
¹²⁹ I	0.46, 0.22	0.63, 0.40	--	--	--	--
²³⁹ Pu	--	0.51, 0.26	--	--	--	--
²³⁸ U	--	0.46, 0.21	--	-0.35, 0.13	--	--
Release from Repository						
Horizontal						
¹²⁹ I	0.86, 0.74	--	--	--	--	--
²³⁹ Pu	--	--	--	--	--	-0.41, 0.16
²³⁸ U	--	--	--	--	-0.39, 0.15	--
Vertical						
¹²⁹ I	0.54, 0.31	0.48, 0.23	--	--	--	--
²³⁹ Pu	--	0.55, 0.28	--	--	--	-0.35, 0.13
²³⁸ U	--	--	--	-0.40, 0.19	--	-0.41, 0.17
Release to Water Table						
Horizontal						
¹²⁹ I	--	--	--	--	--	0.51, 0.26
²³⁹ Pu	--	--	--	--	--	--
²³⁸ U	--	--	--	--	-0.55, 0.28	--
Vertical						
¹²⁹ I	--	--	--	--	--	0.55, 0.31
²³⁹ Pu	--	--	--	--	-0.50, 0.21	--
²³⁸ U	--	--	--	--	-0.49, 0.25	-0.39, 0.15

* Standardized regression coefficient (SRC) of regression mode

** Coefficient of determination (r^2)

TRI-6342-5031-1

Figure 15.7-1. Scatterplots of summed normalized release from the low enriched spent fuel (represented by pressurized water reactor [PWR] fuel—WP 105) versus three sampled parameters that influence the results evaluated by the Simple PA consequence models. (a) release versus minimum infiltration rate, (b) release versus rank of minimum infiltration rate, (c) release versus period of climate change, (d) release versus rank of climatic change, (e) release versus amplitude of infiltration rate (maximum rate minus minimum rate), and (f) release versus rank of infiltration rate.

TRI-6342-5030-1

Figure 15.7-2. Scatterplots of summed normalized liquid release from the repository evaluated by the Complex PA consequence models versus two sampled parameters that influence the results. (a) ^{129}I release versus fraction of containers contacting rubble, (b) ^{129}I release versus rank of fraction of containers contacting rubble, (c) ^{239}Pu release versus effective area for diffusion from disposal container, and (d) ^{239}Pu release versus rank of effective area for diffusion from disposal container.

15.8 Guidance to the Project

The findings listed in the previous section provide the basis for the following guidance to DOE on the potential compliance determination for the waste disposal option under study, i.e., direct disposal of spent nuclear fuel and high-level waste, with minimal treatment or conditioning, in a two-layer disposal container emplaced in a repository in unsaturated tuff.

15.8.1 General Guidance for Waste Treatment Program

In answer to the question regarding what decisions about treatment can be made by DOE before a repository type and site have been identified, the findings suggest that *most decisions on treatment or conditioning should wait until a repository type and site are known. Only those decisions that relate to compliance with current court orders or regulations for storage of high-level waste and spent fuel should be made before a repository site is known.*

This recommendation is based on the finding that minimal treatment of the waste types was sufficient to remain within the reference range defined by the DOE borosilicate glass and the pressurized water reactor fuel, even though a robust (300 to 1000 yr) container was not used in the tuff disposal system.**** The results also showed compliance with current regulations but the absolute position of results is uncertain because full characteristics of the repository and waste are incomplete and the form of future regulations is unknown. This same conclusion was reached for the salt and granite disposal systems in the 1993 PA. This recommendation takes into consideration not only the results of the 1993 and 1994 PAs, but also the expectation of possible changes to the regulations. For example, policies could move from imposing general regulations toward developing site-specific criteria, as suggested in the Energy Policy Act of 1992, Section 801.

Also, it should be noted that the criticality calculations are preliminary and so provide merely an indication of the low likelihood of a critical occurrence. Nevertheless, the calculations appear to support the belief that it would be difficult to create conditions that would provide enough water to (1) corrode the containers (both those with and without a corrosion-resistant material), (2) remove neutron absorbers or uranium, and (3) moderate a nuclear chain reaction within the repository. In addition, a criticality may not be technically disruptive to repository performance.

Little work has been done to establish repository post-closure criticality safety requirements and policy. Thus, there is not as yet a consistent or coherent approach to what technical (risk-based) assumptions can or should be applied in a criticality. Furthermore, methodologies necessary to deal with technical analysis and evaluations (PAs) assignment of risk quantification, probabilistic risk assessments, and criticality calculations need some degree of standardization. Because commercial-type fuel and highly enriched spent fuel have many characteristics in common, cooperative efforts between Office of Environmental Management (DOE-EM), which is responsible for the DOE spent fuel, and the Office of Civilian Radioactive Waste Management (DOE-RW), which is responsible for commercial spent fuel, could be mutually beneficial.

These findings do not mean that characterization of waste is sufficient or complete. Specific recommendations on data needs such as characterization of the waste types, experiments on solubility of radionuclides, and corrosion studies of potential containers that should be pursued to support future disposal are listed under "Recommendations for Future Analysis and Data Acquisition." Even if credit on the license application is taken only for a robust container, some preliminary characterization is expected to be required to assure the regulator that DOE has a rudimentary understanding of its waste. Characterization of the waste would also provide a basis for future treatment of waste, if treatment is considered necessary for acceptance of the waste into a repository.

****The use of a robust container may not be important for the individual dose requirement; rather, a container that fails over a wide range of times may be more useful.

15.8.2 Guidance for Waste Acceptance Criteria

Assuming a total system evaluation, which is consistent with the criteria of 40 CFR 191, the following guidance is given for any waste acceptance criteria.

First, for a repository in unsaturated tuff, disposal of currently existing DOE spent fuel and high-level waste with minimal treatment or conditioning in containers proposed by the Yucca Mountain Project in 1994 will likely show compliance with the Containment Requirements of 40 CFR 191.13. The results also show that waste disposal (1) in a container that does not meet the requirements of 10 CFR 60.113 or (2) in a container that does not meet the waste form requirements in 10 CFR 60.135 could still satisfy compliance requirements of 40 CFR 191.13 for 10,000 yr, and individual dose requirements in 40 CFR 191.15 for 10,000 yr (and even international guidelines on dose using a deterministic calculation up to 100,000 yr at a location 1000 m from the waste using median model parameter values).

Second, no characteristic of the spent fuel owned by the DOE would contribute to a repository in tuff, salt, or granite being less likely to comply with existing regulations than if it contained other spent fuel types, based on the results of the 1993 and 1994 PAs. Issues under study for the DOE-owned waste were criticality and the effects of conditioning. The issue of criticality is important for the DOE-owned spent fuel; however, criticality is potentially important for commercial spent fuel as well (current regulations provide no guidance on the issue of criticality). However, the effects of critical conditions in a repository are not perceptible although the calculations regarding criticality are preliminary and thus cannot be relied upon for final guidance. Also, conditioning does not appear to be necessary for DOE-owned spent fuel with regard to compliance with total system regulations regarding geologic disposal; however, some conditioning of the N-Reactor and Advanced Test Reactor fuel might be necessary to comply with arbitrary release rate limits and waste form requirements in 10 CFR 60 and to improve safety in handling and transportation to the repository.

Third, the combined results of the 1993 and 1994 PAs indicate that the acceptability of the waste form or, alternatively, the need for a container that meets the requirements of 10 CFR 60, in order to meet the overall requirements of 40 CFR 191, is sensitive to the geologic medium of the disposal system (i.e., the type of host rock). Thus, preliminary waste acceptance criteria must clearly indicate the relationship between acceptance and the type of geologic medium in which the repository is located.

15.8.3 Recommendations for Future Analysis and Data Acquisition

The use of performance assessments as a tool during the development and demonstration of the capability to dispose of spent nuclear fuel and high-level waste offers distinct advantages. First, a performance assessment is a valuable and low-cost tool, relative to actual implementation of waste treatment and disposal operations, that responds to the spirit of the Nuclear Waste Policy Act (with amendments in 1987) (NWPA, 1983; NWPA, 1987). Second, a performance assessment is the primary means by which the DOE will demonstrate compliance with long-term environmental regulations and, therefore, should be an essential component of any development program. The INEL Spent Fuel and Waste Management Technology Development Program is unique in recognizing the benefits of a performance assessment early in the program.

In addition to providing guidance to the project, this performance assessment serves to inform both the analysis team and decisionmakers who commissioned the study about (a) the type of model development and analysis that should be conducted in the future and (b) the scientific information that must be gathered, either from the literature or investigative studies, for use in models selected for future performance assessments. Recommendations about model development and analysis can be acted upon by the analysis team; recommendations about gathering additional data may require input from throughout the DOE complex. Both types of recommendations are presented in Tables 15.8-1 and 15.8-2.

Recommendations for Future Model Development and Analysis. The recommendations for future model development and analysis are as follows (Table 15.8-1).

Table 15.8-1. Recommendations for Future Model Development and Analysis**Source-Term and Repository Modeling Development and Analysis**

1. Develop the capability to run simulations that transport oxygen within the repository in order to use both oxic and anoxic corrosion rates and solubility values in the source term model.
2. Continue computations that estimate solubilities of radionuclides in solutions saturated with and without silica.
3. Include an increase of surface area as encapsulating fuel or glass matrix alters over time.
4. Evaluate the effects of the steel and concrete used during the operational phase and left in the repository after closure.
5. Evaluate whether reactants such as oxygen and water are limited significantly to reduce the rate of oxidation of the uranium metal in some types of DOE spent fuel.
6. Develop a version of the source term submodel that can be run separately from the fluid flow and transport codes.

Suggested Criticality Modeling Development and Analysis

7. Examine the corrosion and leaching of borated stainless steel or other material versus the removal of uranium from a container.
8. Examine more uncoupled events to develop an understanding of the feasibility of the critical event in a moderated but unpressurized assembly of fissile material.
9. Continue to examine more of the conditions and assumptions hypothesized in the fault tree for criticality event in or near a waste container.
10. Examine assemblies with larger amounts of fissile material than were used in the 1994 PA to see whether sensitivity to minute changes in saturation is reduced.
11. Examine potential options to lower the probability of critical conditions occurring within the repository.
12. Examine the possibility and consequences of a critical condition at the surface after an exploratory borehole has penetrated the repository and brought fissile material to the surface.
13. Develop the capability to include precipitation of fissile material in transport calculations.

Suggested Geologic Barrier Analysis

14. Compare results assuming a full dual-permeability model to the composite-porosity simplification.
15. Evaluate the possibility of an intrusion borehole enhancing flow above the repository, to a container, and then to the water table.
16. Examine the influence of a weeps conceptual model for flow within tuff.
17. Explore possible ranges for a rise in the water table and its influence on the behavior of DOE spent fuel and high-level wastes.

Suggested Overall Analysis

18. Re-examine the salt and granite disposal options to provide more consistency between the 1993 and 1994 PAs, specifically use the improved source term model from the 1994 PA, and examine the potential for critical conditions developing within or near containers.
19. Compare the advantages and disadvantages of salt, granite, and tuff disposal systems.
20. Evaluate individual doses from the disposal system beyond 10,000 yr.
21. Assess the performance of an unsaturated tuff disposal system containing DOE high-level waste and spent fuel from both public utilities and DOE, since temperature has a large influence on corrosion rates.
22. Evaluate the feasibility of assigning values and ranks to different investigative programs to help allocate program resources.

Table 15.8-2. Recommendations for Data Acquisition

1. Pursue better characterization of the current spent fuel and high-level waste types, specifically, data on spent fuel with regard to failed protective coatings.
 - Estimates of the likelihood of failure of protective coatings on spent fuel in the environment of the repository during the regulatory period.
 - The chemical reactivity of the N-Reactor and Advanced Test Reactor fuels and plans for stabilizing and treating the fuel for storage.
 - The amount of ^{99}Tc and ^{129}I in the calcine high-level waste should be verified.
2. Seek to confirm or develop consensus of alteration rates used in the performance assessment, perform a more thorough literature search and support experiments to obtain temperature-dependent data.
 - For the gas consumption/generation submodel, generalized corrosion rates specific to conditions expected in the tuff repository are needed for the container materials.
 - For the source term submodel, more reliable information about susceptibility and data on failure modes (specific to conditions expected in the tuff repository) are needed for the container materials.
3. Continue to obtain better sorption coefficients used for materials inside and outside the waste parcel (including corrosion products), materials in the unsaturated zone, and materials in the saturated zone.
4. Continue to seek more in-depth information on solubilities of important elements.
 - For the tuff disposal system, these include technetium, iodine, uranium, and neptunium.
5. For the evaluation of critical conditions, obtain defensible release rate of boron from borated steel.

Suggested Source Term and Repository Model Development and Analysis. A possible disadvantage of an unsaturated repository, such as tuff, is that the chemical environment is oxic and thus corrosion rates of protective materials and solubilities of neptunium (Np) and some other actinide radionuclides are greater than in a saturated repository. In the 1994 PA, we assumed that the area around the repository always remained oxic even though large quantities of iron were present, which would be expected to be reducing, especially within the container. Thus, future work should *develop the capability to run simulations that transport oxygen within the repository in order to use both oxic and anoxic corrosion rates and solubility values in the source term model.* This capability would permit a more thorough evaluation of whether reactants such as oxygen and water are limited in reactions within or near the container and thus limit the oxidation rate of uranium metal, the corrosion and alteration of materials, and the solubility of radionuclides. This capability would permit an evaluation of whether materials such as iron, which promote a reducing chemical environment, are useful in terms of waste disposal. Doing so would also allow an examination of the use of filler in the container to further promote a reducing environment.

Several factors affect the solubility of radionuclides, such as (a) the availability of oxygen, (b) the concentration of dissolved silica, (c) pH, (d) precipitation kinetics, and (e) temperature. Because these factors are expected to be markedly different in the far field and within each type of waste parcel, the 1994 PA included two sets of solubilities for uranium, neptunium, and plutonium. Higher solubilities were used for the inside of the container, because silica in the percolating waters there may be removed by reaction with corrosion products, the temperature is higher than outside the container, and there may be less time for formation of more ordered precipitates. Lower solubilities were used outside the container because percolating water there is saturated with silica, the temperature is lower than inside the container, and there is more time for recrystallization of precipitates. This condition, which represents a potential advantage for a tuff repository, needs to be examined in more detail and for other radionuclides. In addition, future analysis should *examine other effects such as the availability of oxygen (Eh) inside and outside the container with the effect of silica saturation, pH, precipitation kinetics, and temperature on radionuclide solubility.*

The surface area exposed to percolating water can greatly increase as the waste matrix alters, and so a minor improvement in the source term model would be to *include an increase of surface area as encapsulating fuel or glass matrix alters over time.*

Besides the waste and containers, a large mass of materials such as concrete and steel could be necessary in the operation of the repository. This material has the potential to alter the chemical environment, and thus future studies

1 should *evaluate the effects of the steel and concrete used during the operational phase and left in the repository*
 2 *after closure.*

3
 4 The chemical reactivity of the uranium metal in the repository is a potential concern. It may be that reactants are
 5 limited sufficiently in a deep geologic repository to maintain a controlled oxidation, much as the nuclear chain reac-
 6 tion was found to be controlled in this year's performance assessment; however, future studies should *evaluate*
 7 *whether reactants such as oxygen and water are limited significantly to reduce the rate of oxidation of the ura-*
 8 *anium metal in some types of DOE spent fuel.*

9
 10 Many of the results reported herein are directly related to the output of the gas consumption/generation and
 11 source term models, which presently run as submodels within the fluid flow and transport codes. To respond rapidly
 12 to design and "what if" questions about the waste forms and to perform sensitivity/uncertainty analyses, it would be
 13 useful to *develop a version of the source term submodel that can be run separately from the fluid flow and trans-*
 14 *port codes.*

15
 16 *Suggested Criticality Modeling Development and Analysis.* Although much was accomplished in the 1994 PA
 17 with regard to criticality, future studies need to perform more calculations to adequately model processes that would
 18 create conditions conducive to a criticality within the repository and its consequences. A key analysis area that needs
 19 additional study is to *examine the corrosion and leaching of borated stainless steel (or other borated material) ver-*
 20 *sus the removal of uranium.* Although some calculations were done, a detailed analysis of the corrosion of borated
 21 stainless steel in the canister inner baskets was not possible given the scope of the 1994 PA. This modeling is neces-
 22 sary to identify whether borated material is leached away from a canister over a 10,000-yr period in amounts substan-
 23 tial enough to be of concern. (Initial calculations indicated that uranium migrated before the boron; see Chapter 10.)
 24 Included in this work would be an analysis to determine the dissolution rate of boron from borated steels in the tuff
 25 groundwater and corresponding material transport. Initially, this modeling should *examine more uncoupled events*
 26 *to develop an understanding of the feasibility of the critical event in a moderated but unpressurized assembly of*
 27 *fissile material* before coupling currently existing nuclear reactor, lumped-parameter codes with current two-phase
 28 flow codes to evaluate dynamics of critical conditions. This analysis can first *continue to examine more of the con-*
 29 *ditions and assumptions hypothesized in the fault tree for criticality event in or near a waste container.* However,
 30 a coupling of fluid flow and nuclear physics can be done without much more effort and should also be attempted
 31 because the end result may be more informative.

32
 33 While the probability of assembling large amounts of fissile material is low, future studies should perform scop-
 34 ing calculations to *examine assemblies with larger amounts of fissile material than were used in the 1994 PA to see*
 35 *whether sensitivity to minute changes in saturation is reduced.*

36
 37 Because the assembly of sufficient fissile material and water for moderation is difficult in the geologic setting,
 38 the addition of a few features in the container or repository could further reduce the probability of a critical condition.
 39 Hence, future studies should *examine potential options to lower the probability of critical conditions occurring*
 40 *within the repository* such as adding filler (internal backfill) within the container to reduce the volume of water avail-
 41 able to moderate nuclear reactions.

42
 43 An additional area is to *examine the possibility and consequences of a critical condition at the surface after an*
 44 *exploratory borehole has penetrated the repository and brought fissile material to the surface.* Because bringing
 45 fissile material to the surface already represents a release, this situation was not examined in the 1994 PA. However,
 46 the critical event should probably be quantified to some extent such that the additional hazards from a criticality can
 47 be compared to the hazard of releasing the contents of a spent fuel container at the surface.

48
 49 A final area to be explored is to *develop the capability to model precipitation of fissile material in transport cal-*
 50 *culations.* Incorporating this capability into current models would be relatively easy; the more difficult aspect would
 51 be constructing numerical models with fine grids, yet reasonable run times, and the proper correlation of solubilities
 52 within and outside the container.

53
 54 *Suggested Geologic Barrier Analysis.* Movement of water in and around the repository is an important phenom-
 55 enon to continue to explore in future studies. The 1994 PA used a composite-porosity simplification in the dual per-
 56

meability conceptual model. A useful step would be to *compare results assuming a full dual-permeability model to the composite porosity simplification*. In addition, the complex behavior in non-isothermal two-phase flow and transport in a heterogeneous fractured porous medium may require models yet to be developed. Involvement in this model development should occur. Enhanced flow from an intrusion borehole was assumed negligible in the 1994 PA because the fracture network was considered to be already permeable. However, scoping calculations should be performed to *evaluate the possibility of an intrusion borehole enhancing flow above the repository, to a container, and then to the water table*. Furthermore, future studies should examine the influence of alternative conceptual models of fluid flow, specifically, *examine the influence of a weeps conceptual model for flow within tuff*. The 1994 PA assumed the influence of a rise in the water table in the first 10,000 yr would be negligible because the change in infiltration was minor over this same regulatory period. However, performing calculations out to 100,000 yr will increase the influence of climatic change and thus the possibility of a rise in the water table. Certainly a large regional model would be necessary to quantify the potential rise in the water table, which might classify this study within the scope of work performed by a specific, potential repository. However, future studies should at least *explore possible ranges for a rise in the water table and its influence on the behavior of DOE spent fuel and high-level wastes*.

Suggested Overall Analysis. Several improvements or changes in the overall analysis should be pursued in future studies. These include *re-examining the salt and granite disposal options to provide more consistency between the 1993 and 1994 PAs, specifically using the improved source term model from the 1994 PA, and examining the potential for critical conditions developing within or near containers* in these disposal systems. A natural addition would be to *compare the advantages and disadvantages of salt, granite, and tuff disposal systems*. Such a comparison can be only qualitative now because of the many changes that occurred between the 1993 and 1994 PAs.

The international community continues to carry out its simulations well beyond 10,000 yr. Although doing so is not specifically required in the United States, the potential benefits of comparing our results with those from other nuclear waste disposal programs throughout the world suggest the need to *evaluate individual doses from the disposal system beyond 10,000 yr*.

Because of temperature's strong influence in a tuff disposal system on the corrosion rates of the disposal container and other protective layers of the spent fuel and high-level waste, specific design goals for temperature are needed for any potential repository. Before these goals become available, it may be informative to *assess the performance of an unsaturated tuff disposal system containing DOE high-level waste and spent fuel from both public utilities and DOE*.

An analysis area that needs improvement is for the results of a performance assessment to become more directly applicable to decisions about programmatic directions. Thus, future studies should *evaluate the feasibility of assigning values and ranks to different investigative programs to help allocate program resources*. For example, the value of characterizing the fraction of particles with failed silicon carbide coatings or claddings on spent nuclear fuel might be ranked against the value of experiments on the solubility of radionuclides in water saturated with silica.

Recommendations for Data Acquisition. Because a need exists for the best, credible data possible in many areas, especially with regard to future licensing applications, specific recommendations for data acquisition with regard to evaluating the performance of DOE spent fuel and high-level waste in a geologic repository are as follows (see also Table ES-15).

The waste treatment program should *pursue better characterization of the current spent fuel and high-level waste types, specifically, data on spent fuel with regard to failed protective coatings* (e.g., fraction of particles with failed silicon carbide coatings is an important model parameter for the graphite spent fuel); *estimates of the likelihood of failure of protective coatings on spent fuel in the environment of the repository during the regulatory period* (e.g., likelihood of failure of silicon carbide coatings of fuel particles in the graphite fuel), and *the chemical reactivity of the N-Reactor and Advanced Test Reactor fuels and plans for stabilizing and treating the fuel for storage*. Based on current regulations, the amount of ^{14}C present and its location (e.g., cladding or UO_2 matrix) in the spent fuel owned by DOE would be pertinent; however, anticipated changes to a standard based on individual doses would eliminate the need for this specific information. *The amount of ^{99}Tc in the calcine high-level waste should be verified* before use in future analysis.

The waste treatment program should also *seek to confirm or develop consensus of alteration rates used in the performance assessment, specifically, perform a more thorough literature search and support experiments to obtain temperature-dependent data. For the gas consumption/generation submodel, generalized corrosion rates* (of, for example, 304L stainless steel, carbon steel, Incoloy Alloy 825, and zircaloy) *specific to conditions expected in the tuff repository are needed for the container materials. For the source term submodel, more reliable information about susceptibility and data on failure modes* (e.g., stress-corrosion cracking, pitting, crevice corrosion, delayed hydrogen-induced failure, and aging reactions) *specific to conditions expected in the tuff repository are needed for the container materials* to adequately assess the longevity of the barrier capabilities of the container.

For credit to be taken for the potential sorption of radionuclides, a waste treatment program should *continue to obtain* (both through literature and experiments) *better sorption coefficients used for materials inside and outside the waste parcel (including corrosion products), materials in the unsaturated zone, and materials in the saturated zone.*

Even accounting for numerous protective layers in spent nuclear fuel, elemental solubility remains important data. Although direct measurements may not be feasible because (1) equilibrium conditions are difficult to reach in lab experiments and (2) the experiments are costly and time consuming because of environmental, safety, and health issues, the waste treatment program needs to *continue to seek more in-depth information on solubilities of important elements. For the tuff disposal system, these include technetium, iodine, uranium, and neptunium.*

For the evaluation of critical conditions, it is important to obtain defensible release rate of boron from borated steel.

Some of the recommendations found in Tables 15.8-1 and 15.8-2 were also raised in the 1993 PA. However, many of the recommendations of the 1993 PA were acted upon this year, including

1. Conducting a performance assessment of a repository in unsaturated tuff, for disposal of spent nuclear fuel and high-level waste, continuing the practice of using different levels of simplification to evaluate consequences. (This assessment required developing a much more versatile source term model and incorporating a composite-porosity model in existing software. The latter improvement allowed two-phase flow and transport modeling in a composite-porosity continuum to be modeled directly in the 1994 PA.)
2. Examining performance criteria other than 40 CFR 191. (In the 1994 PA, we examined the waste package and engineered barrier requirements in 10 CFR 60.135, the individual dose requirements from 40 CFR 191 and international dose guidelines [Volume 3, Appendix D] in addition to the containment requirements of 40 CFR 191.13.)
3. Performing calculations to determine whether the occurrence of critical conditions in a repository would be disruptive to repository performance. (In the 1994 PA, the calculations have covered many different criticality conditions.)
4. Modeling diffusion of contaminants through rubble contacting containers.
5. Acquisition of some data on alteration rates of glass-ceramic matrix and percentage of radionuclides trapped in glass and ceramic phases.
6. Performing geochemical calculations and literature review to obtain a better understanding of element solubility within the repository. (A side benefit was that for criticality calculations, we determined likely mineral phases of uranium that would be precipitated in the repository environment.)
7. Selecting the MPC waste container design of the Yucca Mountain Project as a "reference design" for the performance calculations, although a conceptual LWT container for vertical emplacement was also used.

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Glossary

Acronyms and Initialisms

ALARA – As low as reasonably achievable; principle promulgated by the Nuclear Regulatory Commission (NRC) in 10 CFR 20 that organizations holding NRC licenses should make every reasonable effort to maintain radiation exposures and releases of radionuclides to as low as reasonably achievable.

ATR – Advanced Test Reactor, located at the Idaho National Engineering Laboratory.

BFw – Moderately to densely welded, devitrified ash-flow tuffs belonging to the Bullfrog Member of the Crater Flat Tuff Formation.

BRAGFLO – A computational model (code) that evaluates the simultaneous flow of two phases through a porous heterogenous media.

BRAGFLO_T – A computational model (code) that evaluates the simultaneous flow of two phases through porous heterogenous media. BRAGFLO_T differs from BRAGFLO, its parent code, primarily by the addition of the energy equation for temperature and a much more detailed gas generation submodel; see GASSNF.

CAMCON – Compliance Assessment Methodology CONTroller; computational system for assessing the performance of a disposal system (usually for nuclear wastes).

CCDF – complementary cumulative distribution function; see definition.

CDF – cumulative distribution function; see definition.

CFMn – Nonwelded to partially welded, argillic, zeolitic, and devitrified ash-flow tuffs and minor “bedded tuffs” belonging to the lower portions of the Bullfrog Member and upper portion of the Tram Member of the Crater Flat Tuff Formation. Hydrologic flow and transport properties are assumed to be identical to CFUn.

CFUn – Nonwelded to partially welded tuffs belonging to lower portion of Prow Pass Member and upper portion of Bullfrog Member of Crater Flat Tuff Formation.

Chem Plant – The Idaho Chemical Processing Plant (ICPP); see ICPP.

CHnv – Nonwelded to partially welded, vitric and argillic ash-flow, bedded, and reworked tuffs belonging to the lowermost part of the Topopah Spring Member of the Paintbrush Tuff Formation and the tuffaceous beds of Calico Hills.

CHnz – Similar to CHnv, but consisting of the zeolitized portions of tuffaceous beds of Calico Hills and the non-welded portion of the Prow Pass member of the Crater Flat Tuff Formation.

COND_1D – A one-dimensional thermal-conduction code that provides transient temperature data both inside and outside of a single waste parcel (i.e., both inside the waste parcel interior and in the host rock).

CONRAD – A one-dimensional thermal-conduction and radiation code that provides transient temperature data both inside and outside of a single waste parcel (i.e., both inside the waste parcel interior and in the host rock). The waste parcel and the host rock are assumed to be separated by an air gap.

CUTTINGS – A computational model (code) that calculates the quantity of radioactive material (in curies) brought to the surface as cuttings/cavings by a drilling operation that penetrates the repository. The code determines the amount of cuttings removed from a borehole by drilling and decays radionuclides within the cuttings/cavings to the specified intrusion time.

DHLW – defense high-level waste; the high-level waste, as defined by NWPA §2(12), resulting from reprocessing spent nuclear fuel in a defense facility; the high-level waste considered in this performance assessment.

DOE – U.S. Department of Energy; formed by DOE Organization Act (Public Law 95-91, 912 Stat 565), which replaced the Energy Research and Development Agency (ERDA). ERDA was formed by the 1974 Energy Reorganization Act (Public Law 93-438) and replaced the Atomic Energy Commission (AEC), which was formed in 1946 (August 1, 1946, 60 Stat. 755).

DU – depleted uranium (see definition)

DWPF – Defense Waste Processing Facility (at Savannah River Plant, South Carolina); constructed to dissolve and solidify the high-level waste sludge in borosilicate glass and encasing it in stainless steel canisters.

EB – early defect breach

EPA – U.S. Environmental Protection Agency formed by Congress on December 2, 1970, in Reorganization Plan 3 of 1970 (5 U.S.C. 552, App.; 40 CFR 1). In this act, Congress transfers to EPA the tasks of monitoring research, setting standards, and performing enforcement activities related to pollution abatement and control that allow the environment to be considered as a single, interrelated system.

EPA of 1992 – Energy Policy Act of 1992; an act that requires the U.S. Environmental Protection Agency (EPA) to contract with the National Academy of Sciences (NAS) to recommend site-specific health-based (dose) standards to individuals for the Yucca Mountain Project and subsequent promulgation of new regulations by the EPA and revision of regulations by the Nuclear Regulatory Commission (NRC) consistent with NAS findings.

FFCA – Federal Facility Compliance Act of 1992; an act that removed sovereign immunity for federal facilities concerning hazardous waste regulations; the act requires a listing of mixed-waste inventory at U.S. DOE facilities, and the DOE chose to include spent fuel.

FSV – Fort St. Vrain (graphite moderated reactor in Colorado).

GASSNF – A submodel that calculates the mass rate of gas generation and rate of water consumption. GASSNF is designed as a subroutine of the fluid flow code (i.e., BRAGFLO_T or TOSPAC) and requires liquid saturation of the element as input.

Hanford – See HWVP

HEU – highly enriched uranium; see definition.

HIP – Hot Isostatic Press; process of mixing radionuclides into a glass-ceramic matrix and then compressing the container and mixture as it solidifies; see definition.

HLW – high-level waste; see definition.

HWVP – Hanford Waste Vittrification Plant (Hanford, Washington), designed to immobilize liquid high-level waste stored in double-shelled and single-shelled tanks on the Hanford reservation.

IAEA – International Atomic Energy Agency, Vienna, Austria

- 1 **ICPP** – Idaho Chemical Processing Plant (Idaho Falls, Idaho); located at Idaho National Engineering Laboratory
2 (INEL); also referred to as Chem Plant and operated and managed by Westinghouse Idaho Nuclear Co.
3 (WINCO) from October 1984 through November 1994, and since November 1994, is owned by Lockheed Idaho
4 Technologies Co. (LITCO).
5
6
- 7 **ICRP** – International Commission on Radiological Protection
8
- 9 **INEL** – Idaho National Engineering Laboratory (Idaho Falls, Idaho)
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- 11 **LEU** – low enriched uranium; see definition.
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- 14 **LITCO** – Lockheed Idaho Technology Company, wholly owned subsidiary of Lockheed Corp. Inc., which currently
15 manages facilities at the Idaho Engineering Laboratory (INEL), including the Idaho Chemical Processing Plant
16 (ICPP).
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- 19 **LWR** – light water reactor
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- 21 **LWT** – legal weight truck; in this performance assessment, the LWT indicates a handling container that can be trans-
22 ported by a legal weight truck. The LWT is used for borehole (vertical) disposal; it is placed inside a corrosion-
23 allowance container (overpack). In some simulations, a second overpack, a corrosion-resistant container, is also
24 modeled.
25
26
- 27 **MC₂** – metal carbide (ThC₂, UC₂); interior of the graphite fuel particles.
28
29
- 30 **MCNP** – A general purpose, continuous energy, generalized-geometry, time-dependent Monte Carlo code for neutron
31 and photon transport (Briesmeister, 1986, 1988). The code can also calculate multiplication factor (k_{eff}) eigen-
32 values for a fissile system.
33
34
- 35 **MPC** – multi-purpose canister; in this performance assessment, the MPC is a 125-ton handling container. The MPC
36 is used for in-drift (horizontal) disposal; it is placed inside a corrosion-allowance container (overpack). In some
37 simulations, a second overpack, a corrosion-resistant container, is also modeled.
38
39
- 40 **MTHM** – metric tons of heavy metal
41
- 42 **MTU** – metric tons of uranium
43
- 44 **NEPA** – National Environmental Policy Act of 1969, Public Law No. 91-190, 83 Stat. 852
45
46
- 47 **NRC** – Nuclear Regulatory Commission; formed by the 1974 Energy Reorganization Act (Public Law 93-438) from
48 the Atomic Energy Commission
49
- 50 **NUTS** – Nuclides Transport System (NUTS) is a three-dimensional, multi component, finite-difference, single-
51 porosity, dual-porosity, and dual-permeability simulator to track the movement of radionuclides in the repository
52 and surrounding formations.
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- 55 **NWPA** – Nuclear Waste Policy Act of 1982; provides a national policy for the interim storage, monitored retrievable
56 storage, and eventual disposal of radioactive waste.
57
58
- 59 **NWPAA** – Nuclear Waste Policy Amendments Act of 1987; amendments to the Nuclear Waste Policy Act of 1982
60 specifying that only one repository site at Yucca Mountain was to be characterized by the DOE and placing
61 renewed emphasis on the monitored retrievable storage option.
62
63
- 64 **OCRWM** – Office of Civilian Radioactive Waste Management within DOE; set up to comply with the directives
65 within the NWPA of 1982.
66

Glossary

1 **PA** – performance assessment (see definition)

3 **PB** – Peach Bottom (Reactor 1 and corresponding graphite Cores I and II in Pennsylvania)

6 **PPw** – Partially to moderately welded, devitrified and locally zeolitic ash-flow tuffs belonging to the Prow Pass Member of the Crater Flat Tuff Formation.

9 **PRA** – probabilistic risk assessment (see definition)

12 **PTn** – Nonwelded to partially welded, vitric and locally devitrified tuffs belonging to the lowermost Tiva Canyon Member, Yucca Mountain Member, Pah Canyon Member and uppermost Topopah Spring Member of the Paintbrush Tuff Formation; also includes airfall tuffs, “bedded tuffs,” and intercalated reworked tuffaceous sediments. The Yucca Mountain and Pah Canyon Members are locally welded to the north of the repository region.

18 **PWR** – pressurized water reactor

20 **QA** – quality assurance

23 **RCRA** – Resource Conservation and Recovery Act of 1976 (Public Law 94-580) and, as used herein, subsequent amendments (e.g., HSWA, Hazardous and Solid Waste Amendments of 1984, Public Law 98-616)

26 **RNK** – Repository Nuclear Kinetics is a lumped parameter, transient code to calculate the neutron population (and hence power level) of an assembly as a function of time for a given eigenvalue time history.

30 **Sandia** – See SNL.

32 **Savannah River** – See SRP.

35 **Shippingport** – Experimental Light Water Breeder reactor in Shippingport, Pennsylvania; the reactor was decommissioned in 1986.

38 **SNF** – spent nuclear fuel (see definition)

41 **SNL** – Sandia National Laboratories, a multiprogram laboratory located in Albuquerque, NM, and Livermore, CA. SNL was operated and managed for the DOE from 1949 until October 1993 by Sandia Corporation, which was a wholly owned subsidiary of AT&T. SNL is currently managed by a wholly owned subsidiary of Martin Marietta Corp.

47 **SRC** – standardized regression coefficient in the statistical regression model

49 **SRP** – Savannah River Plant (south of Aiken, South Carolina); originally developed to produce plutonium, tritium, and heavy water for nuclear weapons; the facility of particular interest to this report is the Defense Waste Processing Facility (DWPF).

54 **SS304L** – stainless steel, type 304L

56 **STAFF3D** – As used in this performance assessment, STAFF3D evaluates radionuclide transport through dual porosity saturated media using a finite-element solution technique.

60 **SUMQ_3D** – A three-dimensional code that calculates the time-dependent temperature at any point within an arbitrary array of linear heat sources of finite length; it is limited to providing reliable data outside the backfill-buffer/host-rock interface.

- TCw** – The portion of the Tiva Canyon member of the Paintbrush Tuff Formation that consists of tuffs that are moderately to densely welded, devitrified ash flows.
- TOSPAC** – TOSPAC simulates one-dimensional groundwater flow with the transport of decaying contaminants in partially saturated, fractured media.
- TRw** – Moderately to densely welded, devitrified ash-flow tuffs belonging to the Tram Member of the Crater Flat Tuff Formation.
- TSPA** – Total-System Performance Assessment of the Yucca Mountain Project (YMP), a proposed repository in unsaturated tuff, by the YMP Performance Assessment Departments of the Nuclear Waste Management Center of Sandia National Laboratories. A TSPA was performed in 1991 (Bernard et al., 1992) and in 1993 (Wilson et al., 1994).
- TSw** – Moderately to densely welded, devitrified ash-flow tuffs (including the upper vitrophyre) belonging to a portion of the Topopah Spring Member of the Paintbrush Tuff Formation.
- TSwv** – Densely welded basal vitrophyre belonging to a portion of the Topopah Spring Member of the Paintbrush Tuff Formation.
- UAl_x** – uranium aluminum alloy matrix in special highly enriched spent fuel.
- UO₂** – uranium dioxide; fuel form in low enriched fuel from pressurized water reactor and in highly enriched fuel from Shippingport reactor.
- USATCONC** – A source-term submodel that calculates the dissolution, sorption, and radioactive buildup and decay of specified isotopes within the waste emplacement package. USATCONC is designed as a subroutine to transport codes (i.e., NUTS and TOSPAC).
- WDG** – Waste Disposal Group.
- WEP** – waste emplacement package (see definition)
- West Valley** – See WVDP.
- WINCO** – Westinghouse Idaho Nuclear Company; wholly owned subsidiary of Westinghouse Incorporated which managed the Idaho Chemical Processing Plant (ICPP) at Idaho National Engineering Laboratory (INEL) from October 1984 through October 1994.
- WIPP** – Waste Isolation Pilot Plant; a potential repository near Carlsbad, NM, authorized in 1979 for the management, storage and eventual disposal of waste generated by DOE defense programs that is contaminated with transuranic radionuclides and some RCRA hazardous chemicals.
- WP** – Waste parcel (see definition)
- WPRD** – Waste Parcel Radioisotope Decay software program, which calculates the decay of the inventory of waste in a container. The code is used to evaluate the amount of radioactive material (in curies) brought to the surface by an exploratory drilling operation that hits a waste container. The evaluation includes the assumption that 100% of the original but decayed contents of a container is brought to the surface. WPRD is a simplification of the CUTTINGS code, used by the Waste Isolation Pilot Plant project.
- WVDP** – West Valley Demonstration Project (West Valley, New York)

YMIM – Yucca Mountain Integration Model, written in C++ and developed by Lawrence Berkeley Laboratory, Berkeley, CA, for the TSPA-1993 to evaluate radionuclide concentrations within containers containing low-enriched fuel from pressurized water reactors.

YMP – Yucca Mountain Project; project investigating a potential repository, to be located near the Nevada Test Site, for spent nuclear fuel and high-level waste; under study by the DOE as mandated by U.S. Congress (NWPAA, 1987)

10 CFR 60 – Code of Federal Regulations, Title 10, Part 60, *Licensing Requirements for Land Disposal of Radioactive Waste*

40 CFR 191 – Code of Federal Regulations, Title 40, Part 191, *Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes*

Definitions

absorber – Any material that absorbs or reduces the intensity of ionizing radiation.

accessible environment – "... (1) the atmosphere, (2) land surfaces, (3) surface water, (4) oceans, and (5) all of the lithosphere that is beyond the controlled area." (40 CFR 191.12[k]); the overall performance of the disposal system is calculated at this boundary.

actinide – The series of elements beginning with actinium, atomic number 89, and continuing through lawrencium, atomic number 103; all are radioactive.

activation – The process of making a material radioactive by bombardment with neutrons, protons, or other nuclear radiation (also induced radioactivity).

activity – See radioactivity.

alpha -bearing waste – See transuranic waste.

alpha particle (α) – A type of radiation; positively charged particle (identical to a helium nucleus—two protons and two neutrons) ejected spontaneously from the nuclei of some radionuclides.

alternative conceptual models – Multiple working sets of hypotheses and assumptions of a system that are all scientifically acceptable (i.e., consistent with the purpose of the model, logically complementary to one another, in agreement with existing facts and observed data, and able to be tested).

alternative models – Alternatives in model form that may exist at each stage of model development. Alternatives at the first stage of model development (alternative conceptual models) are often of the most concern.

assembly – A major group of components, e.g., a bundle of fuel rods of low enriched uranium fuel.

Assurance Requirements – Qualitative requirements in Subpart B of 40 CFR 191 (§191.14) that specify actions and procedures to increase confidence that the probabilistic release limits in the Containment Requirements will be met.

backfill – Material used to fill the shafts, access drifts, and other excavated openings. Although not included in the 1994 PA, special types of backfill include concrete and bentonite clay plugs for sealing (seals) and bentonite clay backfill around the waste parcel (backfill-buffer). These types of backfill were included in the granite repository in the 1993 PA.

backfill-buffer – The earthen backfill between the waste parcel and host rock; because some emplacement designs envision using the backfill material to moderate (or buffer) the release of contaminants to the host rock (e.g., bentonite clay in the granite repository), this backfill is also referred to as “backfill-buffer.” The term “backfill-buffer” is used in this report even when the crushed-salt backfill around the waste parcel is discussed, although it does not technically provide a moderating function. The term “buffer” is also frequently found in the literature but is not used here to avoid confusion with the many other uses of the term (e.g., in chemistry, a solution containing a weak acid and conjugate base that resists changes in pH).

barrier – As defined in 40 CFR 191, a barrier “means any material or structure that prevents or substantially delays movement of water or radionuclides toward the accessible environment. For example, a barrier may be a geologic structure, a canister, a waste form with physical and chemical characteristics that significantly decrease the mobility of radionuclides, or a material placed over and around water, provided that the material or structure substantially delays movement of water or radionuclides” (Section 191.12).

batholith – a shield or stock-shaped body of plutonic igneous rock at least 100 km² (40 mi²) in area.

becquerel – SI unit of radioactivity equal to one transformation per second.

bentonite – A common term applied to clay containing montmorillonite (smectite) as the predominate mineral.

beta particle (β) – A type of radiation; a charged (positive or negative) particle emitted from the nuclei of some radionuclides during radioactive decay. A negatively charged beta particle is identical to an electron; a positively charged beta particle is a positron.

borosilicate glass waste – Glass waste from three DOE sites (Savannah River, Hanford, and West Valley) that typically contains 20 to 30 wt% waste oxides, 40 to 65 wt% silica, 5 to 10 wt% boron oxide, and 10 to 20 wt% alkali oxides.

buffer – See backfill-buffer.

burnup – A measure of the consumption of the fissile content of nuclear fuel for reactors; the unit normally used in megawatt-day per metric ton heavy metal (MWd/MTHM).

calcine – Solid, granular, and powdered particles consisting of fission products, trace actinides, and hazardous and nonhazardous materials. Calcine is produced by heating liquid high-level waste and oxidizing components in a fluidized bed.

canister – As used in this report, a canister is equivalent to a handling container. In documents for the Yucca Mountain Project, a canister often refers only to the handling container for high-level waste in borosilicate glass.

cavings – Particulates brought to the ground surface in the drilling fluid of a rotary drill from erosion of the borehole wall by the circulating drilling fluid.

cladding – The outer coating of nuclear fuel, for example, a tube or a plate.

complementary cumulative distribution function – One minus the cumulative distribution function. It is the graphical representation of the probability of exceeding in consequence value $P\{C < C\}$ compared to the consequence value C where for the containment requirements in 40 CFR 191, the consequence value is the sum of the releases (normalized by the EPA release limits) accumulated over 10,000 yr.

Complex PA – A performance assessment that uses consequence models based on a mathematical model with partial differential equations and spatially varying model parameters.

composite porosity mathematical model – A special case of the dual permeability mathematical model where pressure/temperature values in a continuum composed for two media, fractures and matrix, are assumed to be in local thermodynamic equilibrium such that there is no need to separately calculate the pressure and temperatures in the two media. Rather, a single saturation and permeability function, which is a function of properties of the fracture and matrix media, is evaluated. (An arithmetic average of the permeabilities applies for the special case when flow in the fractures is parallel to flow in the matrix.) From the equilibrium pressure, flow results in the matrix and fracture can be obtained through the corresponding capillary pressure curves of the media. Applied by Peters and Klavetter (1988) to a single-phase unsaturated flow and extended by Pruess et al. (1990) to multiphase flow (and called equivalent porosity therein), this mathematical model is implemented in TOSPAC (Dudley et al., 1988) and BRAGFLO_T.

computational model – The solution and implementation of the mathematical model. The solution may be either analytical, numerical, or empirical (where an empirical solution uses observed data directly by means of lookup tables and/or interpolation on statistical relationships). Conceivably, the implementation may be evaluated either by hand or on a computer. However, because the latter is more frequent, computational model is often synonymous with computer model. The computational model is generic until system-specific data are used.

computational scenario – A member of a class of subsets of parameter space that is obtained by subdividing the subspace S spanned by parameters of a summary scenario.

conceptual model – The set of hypotheses and assumptions that postulates the description and behavior of a system. To be scientifically acceptable, the set of hypotheses must be (1) consistent with the purpose of the model, (2) logically consistent with one another, (3) in agreement with existing information and observed data, and (4) able to be tested (i.e., capable of being falsified by the collection of more observed data). At a minimum, these hypotheses and assumptions describe the following about the system, including whether time dependent: (1) the simplified physical arrangement of system components, (2) the initial and boundary condition types, and (3) the nature of the relevant chemical, physical, cultural, or biological phenomena.

Containment Requirements – Requirements in Subpart B of 40 CFR 191 (§191.13) that set probabilistic limits on cumulative releases of radionuclides beyond the “controlled area” (defined in the regulation as a surface location that encompasses no more than 100 km² and extends horizontally no more than a 5-km radius from the outer boundary of a radioactive-waste disposal system, plus the underlying subsurface [§191.12(g)]) for 10,000 years.

controlled area – As defined in 40 CFR 191, Subpart B, “(1) a surface location, to be identified by passive institutional controls, that encompasses no more than 100 square kilometers and extends horizontally no more than five kilometers in any direction from the outer boundary of the original location of the radioactive wastes in a disposal system; and (2) the subsurface underlying such a surface location” (Section 191.12).

coordinate grid or mesh – The grid or mesh on the properly sized modeled object. The coordinate grid is usually called simply the “grid” or “mesh,” except when it is important to distinguish it from the logical grid.

critical condition – A condition in which fission (splitting of nuclei by neutrons) is self sustaining. In the critical (or steady state) condition, just as many neutrons are produced by fission as are lost by sorption and by escape (or leakage) from the system in a given time. The common measure of critical condition is the ratio of the rate of neutron production to the rate of neutron sorption plus neutron leakage; the ratio is symbolized as k_{eff} and called the effective multiplication factor. A critical condition is said to occur when $k_{\text{eff}} = 1$. If the conditions are such that $k_{\text{eff}} < 1$, the system is subcritical; when $k_{\text{eff}} > 1$, the system is supercritical.

critical mass – The smallest mass of fissionable material that will support a self-sustaining chain reaction under specified conditions (e.g., with or without a water moderator).

criticality – A reactor physics term used to describe the state when the number of neutrons released by fission is exactly balanced by the neutron loss mechanisms (neutron sorptions in the assembly and leakage out of the assembly). The reactor (or assembly) is “critical” when it achieves a self-sustaining nuclear chain reaction.

cumulative distribution function (CDF) – The sum (or integral as appropriate) of the probability of those values of a random variable that are less than or equal to a specified value.

curie – A curie is the basic unit to describe the intensity of radioactivity of a material sample. A curie equals 3.7×10^{10} nuclear transformations per second.

cuttings – See drill cuttings.

data – Information that is purposely collected, organized, and used in preparing values for parameters of computational models in an analysis or used as the basis of a decision. As used here, data is a subset of general information.

depleted uranium – The ^{238}U isotope that remains after the fissile ^{235}U isotope has been removed from source nuclear material by isotope separation. Typically, the ^{235}U content ranges between 0.3 to 0.4% by weight in spent fuel compared to 0.7% in natural uranium.

devitrification – Change from a glass to a crystalline condition.

disposal container – See overpack container.

disposal system – Any combination of engineered and natural barriers that isolate spent nuclear fuel or radioactive waste after disposal (40 CFR 191.12(a)). The natural barriers extend to the accessible environment.

dose – The quantity of radiation absorbed accounting for biologic effect; measured in sieverts (Sv) or rem.

drift or access drift – Approximately horizontal underground excavated passageway from the shaft(s) to the mined panels and room(s); in this report, the access drift is 7.62 m in diameter, then backfilled slightly to create a level floor.

drill cuttings – Particulates brought to the surface in the drilling fluid of a rotary drill either from directly cutting through a material with the drill bit or from erosion of the borehole wall by the circulating drilling fluid.

dual continuum mathematical model – See dual permeability mathematical model.

dual porosity mathematical model – A special case of the dual permeability mathematical model where the permeability of the matrix is assumed to be zero such that fluid flow can occur only within the fractures of the two continua. Only diffusion, not flow advection, can occur in the matrix and is orthogonal to the fractures. This mathematical model is implemented in STAFF3D (Huyakorn et al., 1992).

dual permeability mathematical model – A discrete hierarchical model consisting of two continuum, a fracture system and matrix system, that are fully coupled in properties such as pressures of modeled phases, temperatures, and velocities. This mathematical model is implemented in NUTS.

effective continuum model – See composite porosity mathematical model.

Eh – A measure of the oxidizing or reducing tendency of a solution and defined by the Nernst equation, $E_h \text{ (volts)} = E_h^0 + RT/nF \ln ([\text{oxidant}]/[\text{reductant}])$ (e.g., see Freeze and Cherry, 1979, p. 121).

element flaring – The modeling technique of increasing the width (third dimension) of two-dimensional elements according to the radial distance times the desired fraction of a circle, usually a 180° arc. This technique differs from a fully axisymmetric modeling technique in that not all elements are automatically increased in thickness nor are they always increased by the radial distance from one axis times the full 360° circle. Instead, several axes may be used with only a fraction of a circular arc times the radial distance. This technique has been frequently used by the PA Department (since 1990, see Rechar et al., 1990, p. 37) to account for the effective volume (not just area) increase of elements as one moves away from the point of study in a system that is not fully symmetric

(e.g., disposal region of the repository with shafts at one end); in contrast, portions of the study domain with, for example, uniform flow fields do not have the width region increased but instead are set at a constant (e.g., the maximum width of a plume contour).

engineered barrier – Human-designed (engineered) barriers of the waste disposal system. This definition, which is used herein and in 40 CFR 191, includes shafts, boreholes, and their seals. Note that the 10 CFR 60 definition is narrower and omits shafts, boreholes and their seals in its definition.

enriched – An increased percentage of a desired isotope, such as ^{235}U (a fissile radioactive material).

EPA release limits – The normalizing factors for various radionuclides listed in Table 1 of Appendix A of the EPA regulation, 40 CFR 191.

EPA limiting line – The set of lines in CCDF space that connect two limiting points specified in the Containment Requirements (Section 13) of 40 CFR 191. According to the guidance of Appendix B of 40 CFR 191, the EPA can consider a disposal system to be in compliance if the CCDF (predicted by the appropriate probability and consequence models) meets or is less than the two limiting points.

event – A natural or anthropogenic phenomenon that occurs either instantaneously or over a small portion of the time frame of interest.

excursion – A sudden, very rapid rise in the power level of a reactor caused by supercriticality.

feature – An object or condition of the disposal system that influences release of contaminants.

feedback – The return of a portion of the output of a system to the input of a system. Positive feedback enhances the resulting output; negative feedback decreases the resulting output. In the case of a nuclear reactor, an increase in the reactivity of a subcritical fuel assembly to a supercritical (power generating) assembly, without a sufficient cooling system, will result in an increase in temperature. If the system has a large enough negative temperature coefficient, or thermal expansion, the nuclear reaction can be substantially reduced or stopped.

feldspar – Any of a group of crystalline minerals that consist of aluminum silicates with either potassium, sodium, calcium, or barium and that are an essential constituent of nearly all crystalline rocks.

filler – Material placed in the handling container to fill voids, absorb neutrons, or prevent water or other moderating fluid to moderate and help sustain a nuclear chain reaction.

fissile material – Radioactive material fissionable by slow (thermal) neutrons that can produce critical conditions given adequate mass or concentration such that a sustained nuclear chain reaction occurs. The primary fissile materials are ^{233}U , ^{235}U , and ^{239}Pu .

fission – The splitting of a nucleus into at least two other nuclei and release of large amounts of energy. Two or three neutrons are usually released during this transformation.

fissionable material – Any material that can be fissioned by fast neutrons such as ^{238}U . Fissionable material includes fissile material.

fission products – The nuclei (fission fragments) formed by fission of elements and the radionuclides formed from these fission fragments by radioactive decay.

fugacity – An “invented” parameter (f) that measures the chemical potential (μ) of a real gas in the same way that partial pressure (P) measures the free energy of an ideal gas, $f = \gamma(P) \cdot P$, where γ is the fugacity coefficient that varies with pressure for a real gas (e.g., see Castellan, 1971, p. 222).

gamma ray (γ) – A type of electromagnetic radiation of high energy and short wavelength that originates from within the nucleus of the atom. Gamma radiation can accompany some alpha and beta emissions in radioactive decay and always accompanies fission of nuclei.

general environment – Used in 40 CFR 191, Subpart A, as the “total terrestrial, atmospheric, and aquatic environments outside sites within which any activity, operation, or process associated with the management and storage of... radioactive waste is conducted (Section 191.02).

geologic repository – A system intended to be used for disposal of radioactive waste in excavated geologic media. A geologic repository includes (1) the operations area, including both surface and subsurface area, where waste handling occurs, and (2) the geologic setting, i.e., the geologic, hydrologic, and geochemical systems that isolate radioactive waste.

glass-ceramic – Combination of amorphous phase glass and crystalline ceramic material that can bind calcine in the Hot Isostatic Press (HIP) process.

granite – In this report, granite refers to coarse-grained silica-rich igneous rock formed at great depth (plutonic) such as occurs at the Canadian site (Lac du Bonnet, Manitoba) (Everitt and Read, 1989). When modified by a descriptive term, such as “massive grey,” we are referring to a specific granite, essentially of alkali feldspar and quartz.

Groundwater Protection Requirements – Requirements in Subpart B of 40 CFR 191 (§191.16) that set limits on radioactive contamination of certain sources of groundwater within or near the controlled area for 1000 years after disposal.

half-life, radioactive – The time required for half the atoms of a radioactive substance to decay (see also activity).

handling container – The container placed around the waste form or, if the waste form is solidified, the pour container. In some cases a handling container is the sole container for storage, handling, and transportation prior to disposal preparation or disposal itself (see 1993 PA), but in this report the handling container serves as structural reinforcement for subsequent containers (e.g., corrosion-allowance disposal container). The size of the handling container is designated either as LWT or MPC (see related definitions). The handling container is often called a canister.

heavy metal – All uranium, plutonium, and thorium placed *into* a human-engineered nuclear reactor.

high level (radioactive) waste (HLW) – “... the highly radioactive material [fission products and some actinides, atomic number 89-103] resulting from the reprocessing of spent nuclear fuel, including liquid waste produced directly in reprocessing and any solid material derived from such liquid waste that contains fission products in sufficient concentrations ...” (NWPA, 1982, §2[12]). Although not used in this manner in this report, general articles regarding radioactive waste use the term *high level waste* to imply any combination of spent nuclear fuel and HLW (and sometimes transuranic [TRU] waste) that requires disposal in a deep, geologic repository. 10 CFR 60, which was promulgated by the NRC, also includes spent nuclear fuel in its definition of high-level waste.

highly enriched uranium (HEU) – fuel with a content of ^{235}U that is larger than 20% of the total uranium mass; typically used in U.S. Navy propulsion reactors and experimental advanced test reactors.

Hot Isostatic Press (HIP) – Device used to produce temperatures of 1323 K and isostatic pressures of ~140 MPa to produce a monolithic glass-ceramic material binding calcine while mixture solidifies.

implementing agency – The NRC for facilities licensed by the NRC, the EPA for those implementation responsibilities given to the EPA by the WIPP Land Withdrawal Act, and the Department of Energy for any other disposal facility and for implementation responsibilities for the Waste Isolation Pilot Plant not given to the EPA.

Individual Protection Requirements – Requirements in Subpart B of 40 CFR 191 (§191.15) that set limits on radiation doses to members of the public in the accessible environment (the environment beyond the controlled area [§191.12(k)]) for 1000 years of undisturbed performance. (The repromulgation of 40 CFR 191 will likely extend this requirement to 10,000 yr.)

infiltration – Movement of liquid (usually precipitation) at the surface *into* soil and rock. Infiltration is closely related to percolation (flow of liquid through soil and rock) because infiltration can continue only if percolation occurs to remove the infiltrating water at the surface.

internal backfill – Filler placed in the canister or between the canister and overpack to transfer structural and heat loads.

Latin hypercube sampling – A Monte Carlo sampling technique that divides the cumulative distribution function into intervals of equal probability and then samples from each interval.

logical grid – The scaled finite-difference grid of the modeled object such that each cell has unit dimensions, i.e., 1 by 1 by 1. The logical grid is useful for displaying spatial results when cells have greatly varying coordinate dimensions. Because of the irregular connectivity of a finite-element mesh, a logical finite-element mesh is impossible to draw.

low enriched uranium (LEU) – fuel with a higher content of ^{235}U than ore (~ 0.77) but less than or equal to 20% of the total uranium mass; typically used in commercial reactors.

low level waste (LLW) – All radioactive waste other than spent nuclear fuel, high level waste, transuranic waste, and mill tailings. (Mill tailings are the residue from the physical and chemical processing of uranium ore to obtain uranium.) In the United States, LLW is divided into three categories: A, B, and C. Category A has the lowest activity, and Category C has the highest. Some countries create a category called "Intermediate Level Waste (ILW)" by grouping together the U.S.'s Category C LLW, which requires shielding during handling, and transuranic waste.

mass wasting – A general term for the process whereby loosened soil and rock material are transported downslope under the direct influence of gravity either slowly or quickly (e.g., landslide).

mathematical model – The mathematical representation of a conceptual model (i.e., the algebraic, differential, or integral equations that predict quantities of interest of a system and any constitutive equations of the physical material that appropriately approximate system phenomena in a specified domain of the conceptual model. Mathematical models can be categorized as either deterministic or stochastic models).

metric tons of heavy metal (MTHM) – metric tons (1000 kg) of heavy metal (all isotopes of uranium, plutonium, and thorium) before placed into a reactor; the measurement is for initial mass.

model form uncertainty – Uncertainty in the most appropriate model form for a system. The uncertainty results from sparse observed data and lack of information able to corroborate or refute alternative models. Developing alternative models is a way to explicitly acknowledge model form uncertainty; however, in some cases it may be appropriate to combine the alternative models into a megamodel and represent the model-form uncertainty as uncertainty in a parameter.

moderator, neutron – A material such as ordinary water, heavy water, or graphite, that slows down but does not usually absorb high velocity neutrons, thus increasing the likelihood of fission of fissile material.

Monte Carlo – The use of random sampling (and usually computer simulation) to approximate the uncertainty in complex mathematical models.

montmorillonite – A soft clayey mineral that is a hydrous aluminum silicate with considerable capacity for exchanging part of the aluminum for magnesium and bases.

multiplication factor (k_{eff}) – The common measure of critical condition in a finite system. It is the ratio of the rate of neutron production to the rate of neutron sorption plus neutron leakage; the ratio is symbolized as k_{eff} and called the effective multiplication factor. A critical condition is said to occur when $k_{\text{eff}} = 1$. If the conditions are such that $k_{\text{eff}} < 1$, the system is subcritical; when $k_{\text{eff}} > 1$, the system is supercritical.

neutron absorber – A material, such as boron or chlorine, that readily absorbs neutrons and thus reduces the population of neutrons available to cause fissions and thus propagate the nuclear chain reaction.

nuclear chain reaction – A process in which some of the neutron released in one fission event causes other fissions to occur. There are three types of chain reactions: (1) nonsustaining chain reaction—(reactor subcriticality), (2) sustaining chain reaction—(reactor criticality), and (3) multiplying chain reaction—(reactor supercriticality).

nuclear fuel – Fuel containing sufficient fissionable material (material able to split after the sorption or capture of a neutron) to maintain critical conditions in a nuclear reactor.

overpack or overpack container – Secondary container(s) around the handling container of the waste form (i.e., a canister) that provides some specialized function(s) (e.g., corrosion allowance, corrosion resistance, or structural support). In some literature about the proposed repository at Yucca Mountain, an overpack container is called a container barrier assembly.

panel – A grouping of pillars and rooms. Panels are not used in the 1994 performance assessment but were used in the salt and granite repositories for the 1993 PA.

parameters – The underlying fundamental entities ($x = x_1, \dots, x_n, \dots, x_{nV}$) of a computational model. As x changes, so does the model result. The individual parameters, x_n , are usually scalar quantities, but they may also be vectors or functions. Furthermore, the individual parameters are usually coefficients of the mathematical model, but they may also relate to scenario uncertainty or model form uncertainty.

parameter uncertainty – Uncertainty in the most appropriate parameter value for a computational model. The uncertainty results from sparse observed data and lack of information able to corroborate or refute alternative parameter values. Developing distributions of the parameter values is a way to explicitly acknowledge parameter uncertainty; however, in some cases it may be more appropriate to evaluate the computational model at a few possible values of the parameter.

percolation – The movement of liquid (usually water) *through* unsaturated or saturated solid and rock. This flux is directly controlled by the permeability of the medium.

performance assessment (PA) – The *process* of assessing whether a *system* meets a set of *performance criteria*. For this INEL PA, the *process* is a stochastic simulation. The *system* is a deep geologic repository disposal system (volcanic tuff) for DOE spent nuclear fuel, and high-level waste. The *performance criteria* are various long-term environmental metrics in U.S. government regulations (not short-term operational safety issues).

pH – A measure of the proton activity of a solution and equal to the negative logarithm of concentration of hydrogen ions in a solution, $\text{pH} = -\log(c_{\text{H}^+})$

physical process – A natural or anthropogenic phenomenon that occurs continuously or over a significant portion of the time frame of interest.

pillar – A block of rock left intact to support the strata overlying the underground excavations.

poison – See neutron absorber.

probabilistic risk assessment (PRA) – the process of assessing, through a stochastic simulation, the risks from a system. In theory, a PRA is identical to a performance assessment (PA). In practice, the two differ because a PRA usually connotes (a) a system composed solely of human-engineered components, and (b) performance criteria that include risk to health over a short time (e.g., human lifetime) relative to geologic time. A PA usually connotes a system composed of both natural and human-engineered components over geologic time. Because the time frame is different, many phenomena for a PRA can be termed events (short-term phenomena) and, because the components are all human engineered, measured failure rates of components are often available. The modeling tools in a PRA can include elaborate event and fault trees and can substitute empirical data for mechanistic models. For a PA, the event trees are simpler, fault trees are rarely used, and mechanistic models are used directly.

radioactive decay – A process whereby the nucleus of an atom spontaneously emits excess energy by emitting particles (alpha, beta, or neutrons).

radioactivity – The spontaneous emission of alpha or beta particles and/or gamma rays, or emission of x-rays following capture of an orbiting electron from the nucleus of an unstable isotope. Disintegration (decay) of radionuclides per unit time (e.g., 1 disintegration per second is 1 becquerel (Bq); 3.7×10^{10} disintegrations per second is one curie [Ci]).

reactivity – In reactor dynamics, the ratio of increase in the neutron population per neutron generation $\Delta k_{eff}(k_{eff} - 1)$ to the effective multiplication factor (k_{eff}). $\left(\frac{\Delta k_{eff}}{k_{eff}} = \frac{k_{eff} - 1}{k_{eff}} \right)$. A positive reactivity addition indicates a move toward supercriticality; a negative reactivity addition indicates a move toward subcriticality.

reflector – A layer of material immediately surrounding a reactor core that scatters back (or reflects) into the core many neutrons that would otherwise escape.

repository – The portion of a waste disposal facility that includes the waste panels, access drifts, and access shafts. The term “repository” does not include either the above-ground facilities or the undisturbed host rock. (Note that this term differs from the definition in 10 CFR 60 for “geologic repository,” which is described as the disposal system and the current surface facilities.)

reprocessing – The recycling of fissionable material by chemical processing from spent nuclear fuel and refabrication into new fuel elements.

room – An excavated cavity underground for disposal of waste; in this report, a room is a circular tunnel backfilled to create a level floor. The room is 7.62 m in diameter for the vertical emplacement scheme and 4.3 m in diameter for the horizontal emplacement scheme. In the 1993 PA, the room was 9 m wide and 6 m high.

salt – In this report, salt refers to evaporite deposits that are predominantly sodium chloride (NaCl). Mineralogic names such as halite (NaCl), sylvite (KCl), gypsum ($\text{CaSO}_4 \cdot \text{H}_2\text{O}$), and anhydrite (CaSO_4) are used when referring to specific evaporite minerals. The term evaporite includes all of the above minerals; evaporites are formed by the evaporation of a saline solution such as sea water.

scenario – The subset of all features, events, and processes considered for incorporating in the conceptual model of the disposal system. Once a mathematical model of the disposal system has been developed, the term scenario can be more precisely defined in relationship to the parameter space of the mathematical model, i.e., a scenario is a subset of the parameter space defined as a compound statement, $A(\mathbf{x})$, that is built by linking with the conjunction “and” any series of simple statements about values taken by elements of the parameter space, $\mathbf{x}$, and/or the set of consequences, $f(\mathbf{x})$.

scenario screening – A necessary step in the construction of any model of a natural or engineered system in which the phenomena identified through scenario selection are incorporated in a mathematical model of the system.

scenario selection – A necessary step in the construction of any model of a natural or engineered system in which the physical, chemical, and anthropogenic phenomena that *might* play a significant role in determining the performance of the system are identified.

scenario uncertainty – Uncertainty in the most appropriate scenarios for a system. The uncertainty results from omission of discrete, short-term, natural, or anthropogenic phenomena (events), continuous natural or anthropogenic phenomena (processes), and objects and conditions (features) of a system (completeness errors) and the imperfect aggregation of histories of a system (aggregation errors).

seiche – An oscillation of the surface of a lake or landlocked sea that varies in period from a few minutes to several hours.

sensitivity analysis – An analytic or numerical technique for examining the effects of parameters being varied in a model; specifically, an analysis of the effects that parameter changes have on model predictions.

shaft – An approximately vertical or steeply inclined passageway from the ground surface to the underground level of the disposal region. In the 1993 PA, the shaft was 9 m in diameter in salt and 6 m in diameter in granite. In the 1994 PA, long ramps from the surface were included in the design of this hypothetical tuff repository instead of shafts.

Simple PA – A performance assessment that uses consequence models based on a mathematical model with ordinary differential equations and lumped-model parameters; the Simple PA provides a faster model setup and run times compared to a Complex PA, which uses consequence models with spatially varying parameters.

site – As used in this report, the “site” is the general location of the controlled area (the disposal system, including the land surface directly above it). The term “site” also includes any important features surrounding the controlled area (e.g., “site characterization”). Except for the latter addition, this report’s definition of site is most similar to the regulatory definition in 10 CFR 60.2: “the location of the controlled area.” It is roughly equivalent to the regulatory definition of “site” in 40 CFR 191.02, provided “effective control” is loosely defined (e.g., as simply land use or ownership records): “an area contained within the boundary of a location under the effective control of persons possessing or using ... radioactive waste that are involved in any activity, operation, or process covered by this Subpart.”

special spent nuclear fuel (special SNF) – Experimental fuel that originates from many government research and test reactors and non-government research reactors.

spent nuclear fuel (SNF) or spent fuel – “... fuel that has been withdrawn from a nuclear reactor following irradiation, the constituent elements of which have not been separated by reprocessing” (NWP, 1982). In this report, spent fuel can include intact and failed fuel assemblies, consolidated fuel rods, non-fuel components that are a part of a fuel assembly (such as neutron sources, instrumentation, and fuel channels). Although spent nuclear fuel has fissionable ^{235}U , it contains too many radionuclides (primarily short-lived) that adsorb neutrons from the fission process for it to be usefully left in the reactor. Because of spent nuclear fuel’s high value, some countries choose to recycle it (recycling becomes more attractive after the short-lived fission products have decayed away). It is also designated separately from other high level and transuranic wastes in the U.S. Environmental Protection Agency’s standard on disposal of radioactive wastes, 40 CFR 191. In this report, its status as “spent” nuclear fuel, rather than as a “waste,” is maintained when the source of the material is described. However, in the description of the treatment options that specify disposal, it is treated as a “waste” and therefore becomes part of a “waste form.”

subcriticality – The condition of a nuclear reactor system when the rate of production of fission neutrons is lower than the rate of production in the previous generations due to increased neutron leakage and poisons.

summary scenario – A retained scenario from the set of plausible histories of the disposal system. The summary scenario is the result of the scenario selection procedure.

supercriticality – The condition for increasing the level of operation of a reactor. The rate of fission neutron production exceeds all neutron losses, and the overall neutron population increases.

thermal neutron – A neutron that has (by collision with other particles) reached an energy state equal to that of its surroundings.

threshold pressure – In this performance assessment, threshold pressure is defined as the capillary pressure associated with the incipient development of a continuous connection of the nonwetting (gas) phase through a porous medium, providing gas pathways not only through relatively large pore spaces, but also through necks between pores. Thus, threshold pressure (P_t) is the capillary pressure (P_c) at the residual gas saturation (S_{gr}).

transuranic (TRU) waste – Transuranic waste is also termed Alpha-Bearing Waste in some countries. Transuranic waste is contaminated with transuranic radionuclides (atomic number greater than 92) emitting α radiation and having a half-life greater than 20 years and an activity greater than 100 nCi.

tsunami – A long wavelength surface gravity sea wave produced by submarine earth movement or volcanic eruption.

tuff – A compacted or consolidated deposit of pyroclastic ash and dust from a volcanic eruption.

uncertainty analysis – An analytic or numerical technique to evaluate how important the uncertainties of a parameter are (i.e., how likely it is to vary) in explaining uncertainty in the predictions. For example, the results of a model may be very sensitive to varying a parameter, but if the parameter's value is precisely known, the parameter is not important to producing any uncertainty in the prediction. (Uncertainty analysis is sometimes called importance analysis.)

uncertainty propagation – Methods for propagating the uncertainty in parameters of a model, through the model, to calculate the uncertainty in the predictions. Uncertainty propagation is an important aspect of stochastic simulation.

underground facility – The underground structure including openings and backfill materials, but excluding shafts, boreholes, and their seals (10 CFR 60.2).

validation – The process of making valid by confirming, corroborating, substantiating, or supporting, where valid means of good authority, well founded, sound and to the point, and applicable to the subject or circumstances against which few objections can be fairly brought.

validation of an (applied) model – The process of validating through sufficient testing (subjective) using system-specific observed data that a conceptual model and the corresponding mathematical and computational models explain a system with sufficient accuracy (subjective), consistent with the purpose of the model. In other words, model validation is the process of confirming that the applied model is solving the appropriate idealization of the system (correct applied model produced). Verification of a computational model precedes validation of an applied model. Model validation is an ongoing process.

verification of a (computational) model – The process of verifying that a computational model appropriately solves and implements the mathematical model. In other words, model verification is the process of illustrating that the mathematical model is being solved appropriately (computational model correctly produced). Often the computational model is implemented as a code, and verification of the computational model is closely connected to verification of software. Once a computational model is verified, the assumptions of the conceptual model underlying the mathematical and computational model (the applied model) should be validated using system-specific data.

verification of software – The process of illustrating through sufficient (subjective) testing that the software satisfactorily performs its stated capabilities (subjective) and providing a point of reference for future modifications. The extent to which the software can be tested is determined by its complexity.

1 **waste** – The contents of a nuclear waste canister, except any internal filler or neutron absorber packed inside the con-
2 tainer, i.e., high-level waste from reprocessing spent fuel; nuclear spent fuel, brackets and hardware highly con-
3 taminated with radionuclides; and constituents that have been defined as hazardous by the Resource
4 Conservation and Recovery Act (RCRA, 1976).

7 **waste disposal group** – A grouping by similar treatment option of the waste emplacement packages that contain the
8 waste types being considered for disposal.

11 **waste form** – The waste type in combination with a specific treatment option; the form of the waste just before place-
12 ment in a canister. The waste form can often be succinctly described by an adjective summarizing the treatment
13 option (e.g., *shredded* graphite spent nuclear fuel).

16 **waste package or waste emplacement package (WEP)** – According to 10 CFR 60.2, the waste package is “the
17 waste form and any containers, shielding, packing, and other absorbent materials immediately surrounding an
18 individual waste container.” Thus, the waste package contains all components that enclose the waste form out to
19 the host rock. The waste package is defined as a unit as a convenience for subsystem modelers; also 10 CFR
20 60.113(b) places release limits on this unit. In granite, the waste package includes the waste parcel and a clay
21 backfill-buffer around it; in tuff, the waste package and the waste parcel are the same, because only an air gap
22 surrounds the waste parcel. The air gap provides an important protective function and possibly could be con-
23 structed to be part of the waste package.

26 **waste package hole backfill** – See backfill-buffer.

29 **waste parcel (WP)** – The waste form, internal backfill, canister, and overpack. This definition describes a unit that
30 could be handled; it does not include the backfill immediately surrounding the waste package.

32 **waste source** – The source of spent nuclear fuel, e.g., graphite or experimental.

35 **waste type** – A description of the waste that indicates either its spent nuclear fuel source or its type of reprocessing.
36 For this report, examples include graphite spent nuclear fuel, and calcine high-level waste.

38 **zeolite** – Any of various hydrous alumino silicates that are analogous in composition to the feldspars, occur as sec-
39 ondary minerals in lavas and tuffs, and can readily exchange ions of calcium, sodium, potassium, barium, and
40 strontium.