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Revision 6**

**SUPPORT TO THE REVISION OF 40 CFR PART 197
("Yucca Mountain")**

Task 4 - Modeling Uncertainty Effects on a Reference Dose Level

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1.0 INTRODUCTION

This report describes studies to assess the effects of temporal uncertainty over times exceeding 10,000 years on the mean dose of 15 mrem/yr occurring at 10,000 years to the reasonably maximally exposed individual (RMEI) at Yucca Mountain. To conduct these studies, EPA used software submitted by DOE with their comments on EPA's proposed standard issued for public comment in 2005. The DOE software, designated the Peak Dose Model, was a site model designed to evaluate the sensitivity of the peak dose to individuals, caused by various system variables that can affect the long-term performance of the proposed Yucca Mountain repository. This software operates under GoldSim with the Transport Module (see Section 2 for a more detailed description of the Peak Dose Model). The DOE model was modified by EPA to address particular concerns as described in Section 3 below.

The present studies examine the effects on an "edge of compliance dose" from a hypothetical reference disposal system for variations in important model parameters used to characterize the Yucca Mountain site, as they may vary for periods of up to 1,000,000 years (the defined period of geologic stability in the proposed standards). The 15 mrem/yr "edge of compliance dose" at 10,000 years is obtained by modifying the DOE Peak Dose Model software to: 1) include the appropriate radionuclide inventory and engineered barrier performance requirements for determining the starting point for the analyses; and 2) force a limited number of early waste package failures to occur to establish the reference case for the analyses. Using a fixed number of early waste package failures (i.e., within 10,000 years), the sensitivity of the dose to the RMEI from variables of particular interest is then evaluated by setting all other model parameters at their "best-estimate" (typically mean) values, except for the parameters being analyzed for sensitivity. The modified model is designated the EPA Uncertainty Model. This report discusses sensitivity studies conducted with the EPA Uncertainty Model that consider seepage factors, solubility parameters, and infiltration rates on dose to the RMEI.

In essence, the studies indicate how the uncertainty in repository performance changes with times beyond 10,000 years for situations where the mean dose from the repository just meets the EPA individual dose requirements set forth in 40 CFR 197.20 at 10,000 years. The approach taken here removes much of the protection provided by the repository's engineered barrier system (EBS), and focuses on natural system uncertainties and radionuclide solubility uncertainties. To provide the required focus, it was necessary to separate the role of the drip shields and the waste packages from components of the natural barrier system, since the components of the engineered barrier system control the time to failure of the waste containers and the initiation of releases. To accomplish this, drip shields were removed from the model and a limited number of early waste package failures were assumed to occur by some mechanism other than long-term general corrosion.

1.1 REGULATORY BACKGROUND

The Energy Policy Act of 1992 (EnPA) directed the EPA to develop standards for public health and safety specifically for the Yucca Mountain candidate repository site. This action followed closely on the promulgation of the Waste Isolation Pilot Plant (WIPP) Land Withdrawal Act (Public Law 102-579, 1992), which explicitly exempted the Yucca Mountain site from the

provisions of 40 CFR Part 191. Part 191 was first promulgated in 1985 and established generic standards for the geologic disposal of radioactive wastes. In addition to directing the Agency to develop standards specifically for the Yucca Mountain site, the EnPA directed the Agency to contract with the National Academy of Sciences (NAS) to advise the Agency on the technical bases for the Yucca Mountain standards. The EnPA directed that the standards be “based upon and consistent with” the findings and recommendations from the NAS. These recommendations were contained in a report published by the NAS in 1995 (NAS 1995).

One of the recommendations in the NAS report was that compliance with regulatory standards should be judged at the time of maximum risk (i.e., time of peak dose) whenever that occurred (NAS 1995, pg. 2). In promulgating 40 CFR Part 197 (Public Health and Environmental Radiation Protection Standards for Yucca Mountain, Nevada) in 2001, EPA addressed this recommendation by requiring that an assessment of repository releases be performed over a longer period than the 10,000-year time frame for which a regulatory standard would apply, and that these assessments be included in the Environmental Impact Statement that would accompany the license application. In the 2001 standards, a regulatory dose limit would only apply to doses received by the reference receptor over a period of 10,000 years, a compliance test equivalent to that contained in the generic standards in Part 191. This formulation was challenged before the Court of Appeals for the D.C. Circuit. In 2004, the Court ruled that the 2001 standards were not based upon or consistent with the NAS recommendations concerning the time frame for the compliance requirement for the Individual Protection Standard. The Court vacated the standard, “to the extent that it incorporates a 10,000-year compliance period...”¹. This ruling left the Agency with the challenge of developing a regulatory standard that would be applied to the individual peak dose during the geologic stability period, which was defined in the 2001 standards as extending to as long as 1,000,000 years, consistent with the NAS Report.

In Part 191, the regulatory compliance period was limited to 10,000 years. This was based upon a presumption that increasing uncertainties in projecting natural conditions at the site, as well as the performance of the engineered barriers, as time frames advance into the tens to hundreds of thousands of years, would make numerical modeling and projections of possible releases progressively less reliable. There was no presumption in formulating Part 191 that the engineered barriers in the repository would provide total containment of the wastes for all time. Rather, it has always been assumed that engineered barriers would eventually break down and releases from the repository would occur. With the Court ruling, this rationale limiting the compliance period to 10,000 years no longer applies. A longer compliance period covering the geologic stability period was proposed in the draft revision to Part 197, issued in 2005 (10 CFR 49014, August 22, 2005). The assessments presented here were done in response to comments on the proposed standards, particularly as these comments relate to the safety of the repository, the defensibility of the proposed dose limit and, the impact of uncertainties in projecting long-term performance.

Derivation of a numerical dose limit to be applied at peak dose must consider the effects of uncertainties both on setting a dose limit and in determining compliance against that limit. In

¹ Nuclear Energy Institute, Inc., v. Environmental Protection Agency, 373 F. 3d 1 (DC Cir. 2004), U.S. Court of Appeals for the District of Columbia, 2004.

setting a peak dose limit, the question of appropriate levels of health protection is a fundamental concern. Increasing uncertainty in projecting doses to a defined receptor, when time frames stretch into the tens to hundreds of thousands of years, makes the correlation between projected dose levels and actual adverse health effects less reliable. For compliance purposes, there is little practical benefit to setting a regulatory dose limit if little or no confidence can be placed in the assessments of site performance that would be used to judge compliance in the regulatory arena.

The NAS believed that setting exposure limits was a subject for public rulemaking (NAS 1995, pg. 3). The current rulemaking process is addressing this aspect of setting a peak dose limit. The NAS also stated their belief that uncertainties in site characteristics could be addressed through bounding analyses (NAS 1995, pg. 91). At this time, there is an extensive database of site characterization information available for Yucca Mountain, and the increasing modeling capabilities make performing assessments easier and more defensible than in the early 1980s when Part 191 was under development. This situation changes the perspective on the use of performance assessments over very long time periods relative to that in the early 1980s. Keeping these considerations in mind, assessments of the site's very long-term performance can be conducted to judge the effects of uncertainty on projected doses during the geologic stability period. Recently, the Department of Energy (DOE) has released a performance assessment model for the site, which would allow such analyses to be done relatively easily and efficiently. This model is described in the text, along with how it was modified to perform the analyses presented in this report.

The intent of the analyses presented here is to evaluate the effects of increasing uncertainty on performance projections using a site-specific performance assessment model and the available data documented in that model.

1.2 THE YUCCA MOUNTAIN DISPOSAL SYSTEM AND THE ACCEPTABLE PERFORMANCE LIMIT FROM PART 191

The disposal system for deep geologic disposal is designed to contain the wastes for as long as possible and provide controlled release at acceptable levels after the engineered barriers lose their containment capability. The function of the EBS is to contain waste in the repository for as long as practical, i.e., for as long as these barriers can persist and function as intended. The natural barrier performs two functions; one is to provide a relatively stable and predictable environment to support the design and function of the engineered barriers, and the second is to continue to keep releases at acceptable levels through the compliance period once releases from the EBS occur. The disposal system was never expected to keep releases at zero for all time. If it were, dose limits would have been set at zero in Part 191. The 15 mrem/yr mean dose limit represents what was considered acceptable performance for the 10,000-year compliance period. With the challenge of setting a peak dose limit, the question arises as to what an "acceptable" dose might be in the longer time frame of the geologic stability period for the Yucca Mountain site.

The only marker for acceptable performance of a deep geologic disposal system in U.S. regulations is the 15 mrem/yr mean dose limit established in Part 191. This level of exposure is based on a limited compliance period of 10,000 years. A disposal system that delivers doses at

this level meets the compliance limits established in Part 191, but no presumption was made that such a disposal system would, or could, continue to limit releases to this level indefinitely. Therefore, the question can be asked, ‘what would be the impact of uncertainties in the very long-term on estimating the peak dose from a disposal system that just meets the 10,000-year exposure limit of 15 mrem/yr at 10,000 years?’ Many comments received on the proposed standards issued in 2005 criticized the proposed peak dose limit of 350 mrem/yr as a loosening of the 2001 standard, and that uncertainty alone was not a sufficient rationale for departing from the 15 mrem/yr dose limit. The analyses presented here were performed in response to these comments. Our analyses are focused on the role of uncertainty in long-term dose projections to determine if the proposed dose limit truly represents a significant departure from previous standards for geologic disposal, in light of the exceptionally long regulatory time frame represented by the 1,000,000-year geologic stability period defined in the proposed 2005 standards, and the role of uncertainties in projecting performance over very long time frames. The analyses examine two areas of concern for supporting the standard development; (1) how do uncertainties affect the range of projected performance beyond 10,000 years, i.e., do uncertainties increase the range of projected doses as we have assumed in the past; and (2) as an illustrative example of the effects of uncertainties, assess the range of expected doses from a hypothetical disposal system at Yucca Mountain that just meets the 15 mrem/yr dose limit at 10,000 years when that performance is extended through the period of geologic stability, i.e., how do uncertainties affect dose projections for a reference base case. Because of the way the reference case is constructed as explained below, this latter question explores the effects of uncertainties in the natural barrier on dose projections from the hypothetical reference examined.

1.3 THE REFERENCE CASE FOR SAFETY ASSESSMENTS OF THE REPOSITORY

The 15 mrem/yr mean dose limit established in Part 191 serves as a starting point for an examination of projected doses from the Yucca Mountain disposal system, i.e., estimating what would be the performance over the geologic stability period as affected by the uncertainties in the system. In order to interpret the results of such assessments, a reference case (disposal system) must be established so that the dose projections over the very long-term (out to peak dose) can be compared against a fixed starting point. Without a fixed starting point, (i.e., allowing all the variables in the system to change over the analysis period), it would be difficult to impossible to identify what uncertainties in one portion of the system were most responsible for the variations observed in the calculated doses. A simplifying assumption in our analyses is to fix the EBS portion of our reference case, and follow the variations in dose projections considering only the variation in the natural barrier parameters on the dose projections. Sections 3 and 4 of this report describe how the reference case was developed and the analyses performed to explore its performance.

For our reference case we established a hypothetical disposal system at the “edge of compliance”, i.e., one that would deliver a mean dose of 15 mrem/yr to the defined receptor at 10,000 years. This hypothetical disposal system would meet the Part 191 compliance measure. This reference system also addresses comments about “loosening” of the 15 mrem/yr. standard in that we are examining a hypothetical disposal system that would be at the “edge-of-compliance”,

under the range of site conditions expected to operate in the post-10,000 year period. The DOE Peak Dose Model described in the next section of this report offers an appropriate tool to look at the effects of uncertainties in the natural barrier on the projection of doses from the reference case out to the peak dose time. The text in later sections describes how the DOE model was modified to suit the needs of our analyses and the features that make this site model particularly useful for our analyses. A reference disposal system that is functioning at the mean dose level of 15 mrem/yr at 10,000 years would serve as an appropriate starting point against which comparisons could be made for the spread in dose estimates for that fixed reference case followed out to peak dose.

With a greatly expanded compliance period, from the 10,000-year length to the 1,000,000-year length of the geologic stability period, the probability that the EBS will remain totally intact is significantly reduced. Past repository performance assessment analyses by DOE (see Section 5) indicate that even with the highly corrosion-resistant materials used for the waste packages, significant degradation of the EBS can be expected over the stability period. For our analyses the question becomes, what level of performance could develop over this time frame, if we start with the assumption that releases from the disposal system at 10,000 years comply with the 15 mrem/yr mean dose limit? How does uncertainty in dose projections for such an “edge-of-compliance” disposal system behave as the time frame of the performance assessments increases to the time of the peak dose as a function of the inherent uncertainties in the disposal system’s characteristics and behavior?

The analyses presented here attempt to answer the question of how the uncertainties in natural barrier performance in the very long-term manifest themselves in dose estimates for the “edge of compliance” reference case of a disposal system at the Yucca Mountain site. For regulatory decision making, being able to distinguish between alternative conceptual models of the disposal system, (i.e., various selections made for assumptions, mathematical representations, and supporting data which distinguish alternative conceptual models), is an important consideration in both framing standards and making compliance decisions. If uncertainties over the very long-term are very high, the ability to evaluate compliance using dose projections that will vary widely compared against fixed limits is far more difficult than if uncertainties do not result in widely divergent estimates. In a similar fashion, the ability to determine if particular assumptions about site characteristics (e.g., specific solubility limits or retardation coefficients for individual radionuclides), or repository design changes (e.g., thicker waste containers or drip shields) would be dramatically reduced if the inherent uncertainties arising from other portions of the disposal system in the very long-term result in very large spreads in dose estimates from performance assessments. Attempting to distinguish between such alternatives would be difficult to impossible if their specific effects cannot be distinguished within the larger uncertainties of the total system performance estimates. The analyses presented here explore the effects of uncertainties in the natural barrier to determine if they can be shown quantitatively increase or decrease, using an illustrative example a hypothetical “edge-of-compliance” disposal system.

1.4 MODELING THE YUCCA MOUNTAIN DISPOSAL SYSTEM FOR THE EDGE OF COMPLIANCE OVER THE GEOLOGIC STABILITY PERIOD

The geological situation at Yucca Mountain is unique in that the repository is located in an arid environment and in a thick zone of unsaturated rock, thereby limiting the amount of water likely to move through the host rock into the underlying aquifers. The geologic history around the site indicates that past pluvial climate cycles produced wetter conditions in the site area, but were not of such magnitude that extreme changes to the site were produced, such as the development of glacial conditions. This suggests that modeling the site's projected performance under a range of higher precipitation expected in future pluvial cycles could be done with some confidence.

The DOE site model mentioned above and described in more detail in this report allows assessments to be made to evaluate the sensitivity of the disposal system to variations in important variables that exert a significant control over the post-10,000-year performance. This model was developed specifically to do such analyses. It is based on features, events, and processes (FEP) analyses and abstracted models developed for ultimate use in TSPAs. The model has been critically reviewed to determine if it contains the necessary components to reasonably assess the effects of variation in site parameters for the purposes of supporting the rulemaking (SCA 2006).

For our studies, a baseline for a hypothetical disposal system that gives a mean dose of 15 mrem/yr to the receptor at 10,000 years is established. This hypothetical system is then modeled over the stability period to determine the spread in dose estimates at the peak dose time for that fixed system, using the database of site characteristics contained in the DOE model and how uncertainty propagates in the dose projections relative to the dose spread for the initial reference case, i.e., a mean dose of 15 mrem/yr. at 10,000 years. This analysis relies on a site model, which has only recently become available (OCWRM 2005), and a site database contained in that model that reasonably describes the characteristics of the Yucca Mountain repository over the stability period. It should be noted that the analyses presented here are not projections of actual expected performance of the Yucca Mountain disposal system as currently designed but rather are for a hypothetical disposal system. A system with a peak mean annual dose of 15 mrem/yr represents the upper limit of what would be considered an acceptable disposal system according to Part 191 and the proposed dose limit in §197.20. Modeling the behavior of this hypothetical system essentially traces the effects of uncertainties in the long-term on dose estimates for the reference "edge of compliance" system out to peak dose.

2.0 DESCRIPTION OF DOE PEAK DOSE MODEL

2.1 GENERAL MODEL DESCRIPTION

In 2005, DOE developed a simplified peak dose model to evaluate the sensitivity of “representative features, events, and processes [FEPs] that potentially influence the performance of a repository at Yucca Mountain over the period of peak dose...” (OCRWM 2005). This model, referred to hereafter as the DOE Peak Dose Model, included abstractions designed to focus on those FEPs DOE believed to be the most important contributors to peak dose, which is expected to occur hundreds of thousands of years after repository closure. Model elements that might affect doses during the first 10,000 years were excluded if they were not expected to significantly affect peak dose.

DOE states the following:

The simplified model developed for this sensitivity study described in this report is not based on and does not rely upon the Yucca Mountain Total System Performance Assessment model to be developed for the purpose of a license application. It is important to note that the Yucca Mountain Total System Performance Assessment Model is more sophisticated, has far more functionality, and appropriately accommodates many more data inputs than the simplified model described in this report (OCRWM 2005, page 1).

However, the data used for the DOE Peak Dose Model are obtained from numerous Analysis and Model Reports (AMRs)² specifically developed by DOE to support the Yucca Mountain Total System Performance Assessment for the License Application (TSPA-LA). The sub-models comprising the Peak Dose Model are based on reasonable and generally conservative abstractions of the more complex models developed for the TSPA-LA. The DOE modeling approach was, in large measure, based on past modeling activities that have been extensively reviewed by numerous technical experts.

Features of the DOE Peak Dose Model important to the studies described in this report include the following:

- Average infiltration rates were developed for the period of 10,000 to 1,000,000 years using weighted averages based on the duration and infiltration rate for each climate state expected during that period (OCRWM 2005, Table 1). To reflect uncertainty, high, medium, and low infiltration rate assumptions were made. The long-term infiltration rates were determined to be 7.7 mm/yr, 26.6 mm/yr, and 47.6 mm/yr for the low, medium, and high infiltration rates, respectively. The respective probabilities were 24%, 41%, and 35% (OCRWM 2005, Section 6.2.1).

² Most of the DOE Analysis and Model Reports are available online at <http://www.ocrwm.doe.gov/technical/amr.shtml>.

- Only advective transport through the EBS is included. Prior DOE studies had shown that diffusive releases were small (OCRWM 2005, Section 5.2.2).
- The waste forms within the waste packages are conservatively assumed to degrade instantaneously when the waste packages fail due to general corrosion (OCRWM 2005, Section 5.2.4). This conservative assumption is supported by the contention that a significant seismic event is likely to occur over the period up to the peak dose, jeopardizing the integrity of the internal components within the waste packages.
- The DOE Peak Dose Model assumes immediate radionuclide transport through the UZ below the repository and through the fractured volcanic aquifer below the UZ. Only the alluvial rocks in the saturated zone (SZ) are included as a barrier to radionuclide transport in the *base case* (OCRWM 2005, Section 6.2.9). Since the purpose of the DOE model was to examine the sensitivities of the disposal system with regard to the peak dose projections, this simplification is consistent with the intent of the DOE modeling effort. Retardation in the degraded waste form and in the drift inverts in the drifts is included in the model.
- Emplacement drift seepage, which depends on percolation flux, fracture permeability, and capillary strength, is based on properties of collapsed drifts. Under this conservative assumption, the effective footprint for the collapsed drifts is twice the size as for the non-collapsed drifts, doubling the percolation flux available for radionuclide transport (OCRWM 2005, Section 6.2.2; BSC 2004, p. 6-29).
- The model includes only those radionuclides expected to be significant contributors to peak dose (OCRWM 2005, Section 6.2.6). Biosphere dose conversion factors (BCDFs) for these nuclides are based on ICRP Publication 72 methods (ICRP 1996).

Switches on the model dashboard permit the code user to examine the sensitivity of the following variations to the model *base case*:

- Igneous intrusion
- Seismic mechanical damage
- Deterministic infiltration rate (low, medium, or high)
- Non-collapsed drift seepage
- Np solubility control
- Removal of drip shield
- Full general corrosion temperature dependency of waste package corrosion rate (allowed to fall to 21° C, instead of being cut off at 45° C)
- Length of the SZ
- Waste package corrosion rate accelerated by factor of 5
- Drip shield corrosion rate accelerated by factor of 5

These features are included in the DOE software for the Peak Dose Model. As will be discussed in this report, EPA modified the software to provide additional capabilities for conducting sensitivity studies of particular interest to the Agency.

2.2 INTEGRATION OF DOE PEAK DOSE MODEL AND GOLDSIM

The DOE Peak Dose Model was implemented in GoldSim, Version 8.02. GoldSim³ is a general-purpose and highly graphical probabilistic simulation framework with specialized modules to support mass transport modeling. It is an object-oriented program, which facilitates the development of models built by linking pre-constructed model elements. Optionally available modules contain elements specifically designed for ground-water pollution simulation studies. With the Radionuclide Transport Module, the program has the capability to model the flow of water through a system of ground-water pathways and track the movement of radionuclides after a breach of containment. In the DOE Peak Dose Model, specific characteristics of the local ground-water pathways, waste package containers, engineered barriers, and important radionuclides are provided to the model in the form of lookup tables. The data in these tables were derived from various DOE AMRs prepared to support the TSPA-LA and referenced in OCRWM 2005. The model also includes stochastic elements designed to reflect the uncertainty and variability in the model parameters. Due to fundamental changes made in more recent versions of GoldSim, the DOE Peak Dose Model and the EPA Uncertainty Model can only be run using Version 8.02.

2.2.1 The DOE Peak Dose Model and DOE *Base Case*

The DOE Peak Dose Model traces the flow of water from the surface through the UZ above the repository, past the drip shields, into the waste packages, through the waste storage drifts and invert, and then through the SZ and alluvium in the Amargosa Valley down-gradient from the repository to a point where individuals receive doses from water drawn from wells.

The timing of waste package failures is provided exogenously. DOE uses a detailed set of Excel spreadsheets to model the effects of general corrosion on the drip shields and waste packages. These spreadsheets produce a distribution of failure times, which is entered into the model in a set of lookup tables and GoldSim stochastic elements. The waste package failures always occur after 400,000 years in DOE's *base case* model. The DOE model also includes separate analyses for igneous and seismic scenarios. These capabilities were not used in the current studies because they represent disruptions of the disposal system performance rather than the evolution of disposal system performance over time, which is the focus of EPA interests. In particular, probability-weighted doses for igneous scenarios contribute only small additional increments to the undisturbed case profile over the period of geologic stability (BSC 2001). Also, the effects of seismic events are implicitly covered in the seepage analyses in Section 4.2 below, since drift collapse is a major possible consequence of seismic activity.

GoldSim data elements include interfaces with Excel spreadsheets. The original DOE Peak Dose Model did not make use of this feature. Although many input tables were derived using spreadsheets, the results were "hardwired" into the GoldSim code. In the EPA studies, a specially created Excel spreadsheet *SelectValue.xls* is used to control the values of the stochastic

³ For more information on the use of GoldSim for modeling at Yucca Mountain, visit their website <http://www.goldsim.com/>.

data elements GoldSim uses in each realization (see Section 3.1 of this report). When needed, the spreadsheet can pass the mean value of the parameter back to GoldSim for use in each realization. The spreadsheet has many other options as well, such as selecting the median or other percentile of the distribution, or a random value that is within one standard deviation of the mean. Sensitivity runs for the EPA studies were conducted by holding one set of parameters at their mean values, while permitting other parameters to range over their entire distribution.

Each uncertain or variable parameter is assigned a probability distribution within a stochastic element. There are over 100 variable parameters in the DOE Peak Dose Model. Due to the presence of these stochastic elements, many different outcomes are possible. The model is run for a large number of realizations (usually 1,000) to capture the wide spread of possible outcomes. In the EPA studies, the stochastic parameters may be fixed at their mean value. If all parameters are fixed at their means, only one realization is necessary. However, if one or more parameters are permitted to vary, then multiple realizations are required. The model, as provided by DOE, takes approximately 1 hour to run in Windows XP on a Compaq Presario desktop computer using a 3400⁺ Athlon 64 processor at 1.8 GHz with 2 GBytes of RAM. The model, as modified to support the EPA studies with the added fixed parameter spreadsheet interface, takes around 100 minutes to run 1,000 realizations. Output files are large, generally of the order of 80 MBytes.

DOE developed a *base case* for the DOE Peak Dose Model against which sensitivity comparisons of interest to the Department could be made. The *base case*, which uses time steps of 5,000 years, "...consists of 1,000 realizations to project future repository performance without considering the consequences of seismic mechanical damage, igneous intrusion, and igneous eruption. Values of uncertain parameters are sampled and repository performance is evaluated over a 1,000,000-year period based on the value of those sampled parameters. Results are presented in terms of the arithmetic mean annual dose, the median annual dose, and several percentiles of the annual dose (OCRWM 2005, p. 125).

As shown in Figure 1,⁴ the DOE Peak Dose Model *base case* produced a mean peak dose of about 125 mrem/yr at 730,000 years; the median peak dose of about 42 mrem/yr occurred at 865,000 years (OCRWM 2005, Figure 13). DOE notes that the mean peak dose is dominated by Pu-242 and Np-237 (OCRWM 2005, Section 6.3.1).

⁴ The sources for the figures and tables in this report refer to the Run ID from Appendix B, Tables B-1 and B-2, which summarize the changes made among model runs.

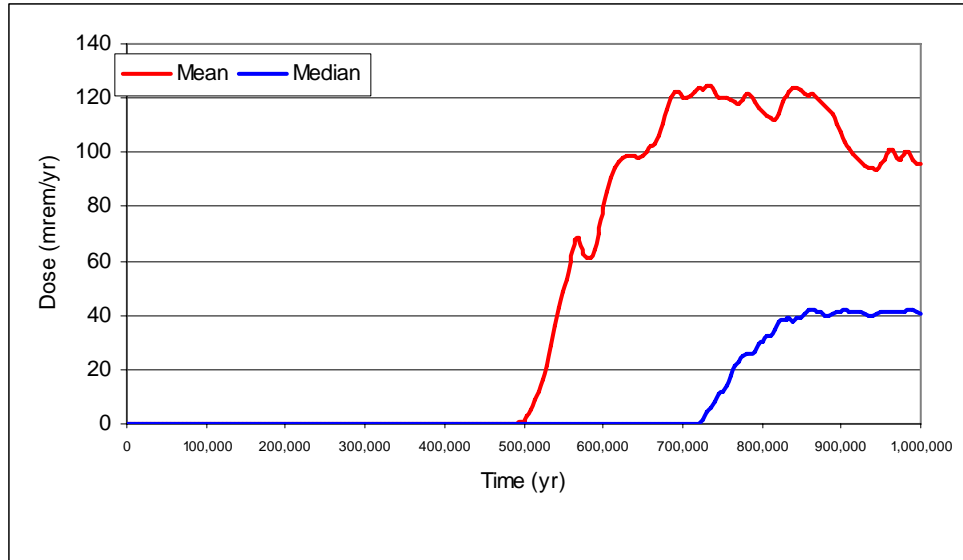


Figure 1. Mean and Median Doses for DOE Peak Dose Model *Base Case*
(Source: Run 14)

2.2.2 Uncertainty and Variability

The terms uncertainty and variability are used commonly in safety assessment, often interchangeably, although their meanings and implications are quite distinct. Variability strictly refers to the variation in the characteristics of the natural and EBS materials as measured by field and laboratory investigations. Characterization of the properties of man-made materials can be performed with considerable rigor, and the variations in these properties can be precisely measured for the most part. Characterizing the natural barrier is considerably less precise because of the heterogeneity of the natural system and the difficulties in controlling all the variables that affect the parameters of interest. For example, the thermal properties and behavior of a metal waste container can be determined much more precisely than the hydraulic conductivity field across a hydrologic unit near the site, or the retardation factors used to describe radionuclide transport along the migration pathway through the natural barrier.

For the long-term safety assessments of the geologic disposal system involved here, a database of relevant parameters must be available and must reflect not only field and laboratory measurements (variability), but an estimation of how these properties vary over the extremely long time frames involved in projecting repository performance (uncertainty). The Yucca Mountain site database built into the DOE Peak Dose Model represents the product of an exhaustive characterization program around the site, extending back to at least 1988 when site characterization efforts increased dramatically with the passage of the Nuclear Waste Policy Amendments Act. The Yucca Mountain site database contains the data generated from field and laboratory investigations, as well as estimates of how the characteristics of the site may vary over long time frames, estimates that rely significantly on professional judgment of the scientists involved in the DOE program over this time period. This database is used in the assessments reported here without any attempt to further manipulate or modify the data. In several instances,

DOE extrapolated data in the AMRs that were limited to 10,000 years to the longer time periods used in the Peak Dose Model.

These data represent the melding of the two aspects—variability and uncertainty. The parameter distributions in the DOE Peak Dose Model reflect both the measured variability in site characteristics, as well as estimates of how these data may vary over the time frame of the geologic stability period. For example, the infiltration data shown in Figure 2 represent variability in the range of infiltration data based on site investigations (plotted along the y-axis of the graph for the present day (time 0)). The remaining data shown on Figure 2 represent uncertainty in that they are estimates of what the ranges of infiltration may be over the course of the stability period based upon other information from which infiltration could be inferred.

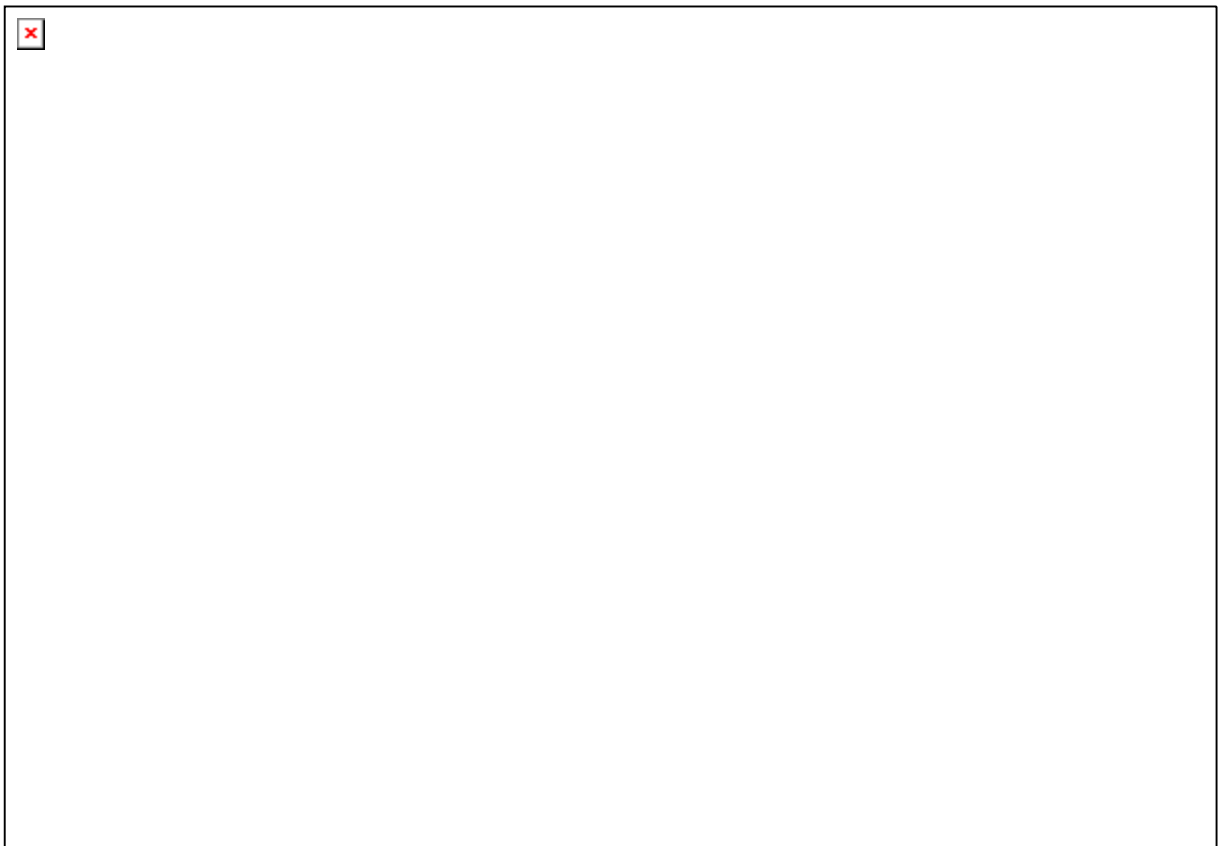


Figure 2. Infiltration Rate Functions for EPA Modeling Studies Based on Tables 1 and 2 of OCRWM 2005

(The high, medium, and low cases have probabilities of 0.35, 0.41, and 0.24, respectively.) (Source: Run 1)

In some cases, individual stochastic elements in the DOE Peak Dose Model are clearly identified as sources of variability or uncertainty. For example, the distributions assigned to the fracture permeability and capillary strength parameters (k_{lith} , k_{nonlith} , and $one_over_alpha_A$) reflect uncertainty concerning these parameters. These seepage parameters are found to be among the five most important parameters for explaining the variability of the model forecasts. The seepage rate and seepage fraction computed from these stochastic elements are then adjusted to account for spatial variability using factors that depend on the infiltration rate parameter (OCRWM 2005, Table 26).

Another highly important stochastic parameter is plutonium solubility (*Log_Pu_Sol_eps1*), which reflects uncertainty in the thermodynamic data for plutonium. A related parameter (*Log_Np_Sol_eps1_NpO2*) reflects similar uncertainties in the thermodynamic properties data for neptunium. The solubility models for plutonium and neptunium also include four additional uncertainty elements (*Log_Pu_Sol_eps2_CDSP*, *Log_Pu_Sol_eps2_CS NF*, *Log_Np_Sol_eps2_NpO2_CDSP_I*, and *Log_Np_Sol_eps2_NpO2_CS NF*) that reflect uncertainty in fluoride concentrations in the percolating water. Similar approaches are applied for protactinium, thorium, and uranium solubility uncertainties.

We will describe some of the assessments of projected performance using the term uncertainty assessments, since they use the full range of parameter values in the database and include both uncertainty and variability. This report also presents the results of sensitivity analyses—i.e., calculations where parameter values were fixed (at mean values) and selected parameters were allowed to vary over their assigned distributions to assess the effects on the peak dose. The intent of these sensitivity analyses is to illuminate what the significant “driver” parameters are for the fully stochastic assessments, and to help interpret their implications on the fully stochastic estimates of peak dose.

2.3 DOE PEAK DOSE MODEL SENSITIVITY STUDIES

DOE described several sensitivity studies using the Peak Dose Model (OCRWM 2005, Section 6.4). Comparisons were made against the results of the nominal *base case* scenario that yielded results similar to those shown in Figure 1 of this report. In addition to the sensitivity analyses summarized below, DOE also evaluated the sensitivity of the drip shield and waste package corrosion rates. However, these results are not discussed here, since the issues of greatest interest to EPA in the present study did not include the performance of the EBS.

DOE’s sensitivity studies focused on both engineered and natural barrier components and their influence on the peak dose estimates. In our approach, we assume that the engineered barrier has lost its containment function to the extent that the disposal system is performing at the regulatory limit (15 mrem/yr) at 10,000 years, and we follow the performance of this system out to the time of peak dose. As explained in more detail in Section 3, we do not include additional waste package failures in the post-10,000-year timeframe. Therefore, DOE’s engineered barrier sensitivity studies are not of direct relevance to our approach. DOE also examined the effects of variables in the natural barriers that strongly influence peak dose estimates, as described below.

2.3.1 Infiltration Rate Sensitivity

DOE compared the results of High (47.6 mm/yr) and Low (7.7 mm/yr) infiltration rates with the *base case* results. It should be noted that in the DOE Peak Dose Model, the percolation flux at the repository horizon is the same as the infiltration rate. To make this comparison, DOE made a run of 1,000 realizations, where all parameters except infiltration rates were allowed to vary over the full range. In this run, 500 realizations were at the high infiltration rate and 500 were at the low infiltration rate. The results showed that the peak mean annual dose at the high infiltration rate was increased by 29% over the *base case*. The peak mean annual dose for the low infiltration rate was 35% lower than for *base case* (OWRWM 2005, Figure 27).

2.3.2 Seepage Sensitivity

In the seepage sensitivity study, DOE compared the *base case* in which drifts were assumed to have collapsed with a case where drifts were assumed to remain intact. To accomplish this, seepage response surfaces for collapsed drifts were replaced with seepage response surfaces for non-collapsed drifts. These response surfaces are look-up tables that display mean seepage flow rate (kg/yr/waste package) and seepage fraction⁵ for high, medium, and low infiltration rates as functions of fracture permeability and capillary strength. These response surfaces are provided in Appendix A of OCRWM 2005.

The DOE Peak Dose Model includes several parameters that determine the amount and location of seepage of ground water onto the waste packages. These include capillary strength, fracture permeability, and flow focusing. The capillary strength parameter ($1/\alpha$) is a measure of the ability of the fractures in the host rocks to contain the ground water in the crown of the drifts and prevent it from dripping on the waste packages. DOE proposed four different methods for determining capillary strength (OCRWM 2005, Table 4), but used only Method A, since the results were not sensitive to variations between the methods. Method A includes both spatial variability and parameter uncertainty.⁶ Distributions assigned to these capillary strength parameters are the same for both lithophysal and non-lithophysal rocks in Method A. Tangential fracture permeability in the boundary layer adjacent to the drifts can divert water around the drifts and prevent it from impinging on the waste packages. As with capillary strength, fracture permeability has components of both spatial variability and parameter uncertainty. Different distributions are assigned to lithophysal and non-lithophysal rocks (OCRWM 2005, Table 5).

The DOE Peak Dose Model also includes a flow-focusing parameter, which accounts for effects of heterogeneity in UZ flow above the repository. This parameter is assumed to vary uniformly from 1 to 2. The DOE Peak Dose Model *base case* assumes seepage parameters associated with collapsed drifts. In collapsed drifts, both the seepage fraction and seepage rate are greater than for non-collapsed drifts.

This DOE sensitivity study showed that changing from the conservative assumption of collapsed drifts to the assumption that the drifts had not collapsed reduced the peak mean annual dose by 70%. DOE concluded, “Since the peak annual dose is dominated by advective radionuclide transport processes, changes in both the fraction of waste package locations contacted by seepage and the corresponding seepage rates have a significant effect on the result measured by both the arithmetic mean and the median” (OCRWM 2005, Section 6.4.2).

⁵ The mean seepage rate is the percentage of the percolation flux that enters a drift over an area defined by the drift width and the waste package length (OCRWM 2005, Section 6.2.2). The seepage fraction is the fraction of the total number of waste packages contacted by water dripping into the drifts.

⁶ Although Method A includes a spatial variability distribution, this distribution is not used in the DOE Peak Dose Model. Instead, DOE uses a multiplier (the seepage parameter adjustment factor shown in Table 26 of OCRWM 2005) to account for spatial variability. The adjustment factor depends only on the infiltration rate—high, medium, or low.

2.3.3 Saturated Zone Sensitivity

As described in Section 2.1, the DOE Peak Dose Model considers only the alluvial portion of the SZ below the Yucca Mountain repository as a barrier to radionuclide transport. Transport through the UZ below the repository and the fractured volcanic rocks in the SZ is conservatively assumed to be immediate upon release of radionuclides from the EBS. DOE analyses showed that the output (g/yr) from the alluvium of strongly sorbing radionuclides, such as Pa-231, Th-229, and Th-230, was reduced by 1 to 3 orders of magnitude as compared to the input to the alluvium, while for Pu-242 and other plutonium isotopes, the mass transport rate was reduced by about 25%. The mass transport of non-sorbing Np-237 was essentially unaffected by passage through the alluvium (OCRWM 2005, Section 6.4.5).

To further demonstrate the importance of the alluvium in reducing doses to the RMEI, DOE conducted a sensitivity test where the alluvial pathway length was set at essentially zero. (This, of course, is an extreme variation that is not reflective of expected physical reality at the repository over the period of geologic stability.) In this case, the mean peak dose was about a factor of 20 higher than the mean peak dose for the *base case*. Radionuclides that are strongly sorbed by the alluvium, such as Th-229, Pa-231 (and its secular equilibrium daughter Ac-227), and Th-230 (and its secular equilibrium daughter Ra-226), are the principal contributors to the increased dose for the case with no alluvium. The Pu-242 dose contribution increases about 45% and the Np-237 contribution is unchanged (OCRWM 2005, Section 6.4.5). DOE states, “These results demonstrate the importance of the natural barrier system below the repository, in particular the alluvium portion of the SZ, over the period of peak dose. The inclusion of the UZ below the repository and the fractured volcanic aquifer portion of the SZ in a fully integrated system level model would result in lower projections of the peak annual dose” (OCRWM 2005, p. 160).

2.3.4 Neptunium Solubility Sensitivity

In the Peak Dose Model *base case*, DOE assumed that NpO_2 was the solubility-controlling phase for neptunium. An alternative solubility model was also evaluated which assumed that the neptunium is incorporated as a solid solution in a secondary uranium mineral formed by the reaction of uranium oxide in the spent fuel with seepage water. DOE found that, with the alternative solubility model, the mean peak dose was reduced by 12% as compared to the *base case*. The contribution of Np-237 to the mean peak dose was reduced by about 50%. DOE concluded, “...the choice of the Np solubility-controlling phase (NpO_2 or secondary phase control) does not significantly affect the annual peak dose for the current peak dose model...” (OCRWM 2005, Section 6.4.3.2). DOE also notes that the neptunium solubility controls become more important at lower seepage rates.

3.0 DEVELOPMENT OF THE EPA UNCERTAINTY MODEL

3.1 INTRODUCTION

This section describes the changes made to the DOE Peak Dose Model to address the question of how a disposal system at the edge of compliance at Yucca Mountain at 10,000 years would perform out to the time of peak dose. The “edge of compliance” disposal system was analyzed to understand how the natural barriers—an essential part of the proposed Yucca Mountain repository—would perform, and how these barriers would contribute to long-term uncertainty in repository behavior, as reflected by the spread of dose projections. To accomplish this goal, it was necessary to modify the DOE Peak Dose Model to remove the influence of two key engineered barriers—the waste package containers and the drip shields—that control the initiation of releases from the repository. This is consistent with the idea that, at some time, the EBS would fail and doses would be largely controlled by the performance of the natural barrier. As noted previously, the modified DOE Peak Dose Model is called the EPA Uncertainty Model.

The approach to creating the “edge-of-compliance” system in the EPA Uncertainty Model was to assume non-corrosive failure of a limited number of waste packages within 10,000 years after repository closure. It should be emphasized that the EPA Uncertainty Model is not designed to predict the long-term performance of the actual Yucca Mountain repository. Rather it is intended to explore the range of possible performance of a hypothetical repository at the Yucca Mountain site that just meets a mean dose criterion of 15 mrem/yr at 10,000 years, using various parameters associated with the natural system and excluding engineered barriers. Since the “edge of compliance” system is a hypothetical construct and not a simulation of the actual expected disposal system performance, the projected ranges of peak dose should not be interpreted as projections of the expected performance of the repository, which in reality will be different since the complex corrosion processes and release mechanisms involving the metal containers and drip shields are considered in actual TSPA calculations. In addition, the results of these assessments should not be interpreted as meaningful projections of the time of the peak dose for the repository performance. However, these times are useful for comparisons of runs in the sensitivity studies, described in more detail in Section 4 of this report, where the effects of variations in individual parameters are examined.

3.1.1 Modifications to the DOE Peak Dose Model to Create the EPA Uncertainty Model

Several changes to the DOE Peak Dose Model were necessary to remove selected features of the EBS. The model, as received, contains a checkbox that permits the model user to remove the drip shield functionality. Intact drip shields prevent seepage from contacting the waste packages for periods of over 100,000 years. This checkbox is checked in all runs of the EPA Uncertainty Model, removing the drip shields from the flow path.

After removal of the drip shields, the waste package containers would still function to prevent water from contacting the waste for several hundred thousand years. Hence, it was necessary to replace the general corrosion module for waste package failure with a waste package failure module that permits failures within the first 10,000 years. This was accomplished by hypothesizing that a selected number of waste package containers would fail at a uniform rate

over the period of 0 to 5,000 years with the drip shields removed from the system. (Travel times for non-sorbing radionuclides from the repository to the RMEI are projected to be on the order of 5,000 years (Edderbarh 2001)). The early waste package failure times were inserted in the model as an alternative for the general corrosion model-based estimates of waste package failure times. This change was introduced in a way that permits the EPA Uncertainty Model to run in either of the following modes:

- (1) Assumed *early failure mode*, with a user-specified number of waste packages that all experience early failure in the first 5,000 years
- (2) *General corrosion failure mode*, with all 11,184 waste packages that are subject only to general corrosion failures, which occur much later following the DOE waste package failure model.

To spread the occurrence of the selected number of early failures over the 5,000-year period, the length of the time steps used in the early time periods was shortened to 500 years. Certain features of the EBS were retained, including retardation of radionuclides by corrosive products in the failed waste packages and in the invert.

The approach to early failures used in the EPA Uncertainty Model should not be confused with the approach taken by DOE in various TSPAs. In the EPA model, a sufficient number of waste packages are forced to fail in less than 5,000 years to produce a mean dose to the RMEI of 15 mrem/yr at 10,000 years. In the TSPA for Site Recommendation (TSPA-SR), DOE assumed that a few waste packages would fail early from manufacturing defects, but these failures resulted in no releases of radioactivity for the first 10,000 years (BSC 2001, Figure 3.2.5.4.1). Subsequently, in the TSPA developed for the 2001 Supplemental Science and Performance Analyses, DOE assumed that early closure weld failures due to improper heat treatment could occur in one or two waste packages. Such failures would produce a mean dose of about 0.008 mrem/yr at about 6,000 to 7,000 years (BSC 2001, Figure 3.2.5.4.1).

The next step in developing the EPA Uncertainty Model was to add I-129 and Tc-99 to the DOE Peak Dose Model. While these species had been included in earlier DOE TSPA models, they were eliminated by DOE from the Peak Dose Model as not being significant contributors to peak dose (OCRWM 2005, Section 6.2.6). However, since EPA's interests include earlier times in order to set up the edge of compliance system at 10,000 years, these species were included in the EPA Uncertainty Model. Solubility data for Tc-99 and I-129 were obtained from BSC 2004a (p. 124), inventory data were obtained from BSC 2004b (Table 7-1), and dose conversion factors were obtained from BSC 2005 (Table 6.2-13). Partitioning coefficients (K_d 's) for these species were set to 0 in the alluvium (BSC 2004d, Section 6.5.3.1) and the invert (BSC 2004e, Section 6.3.4.2.2). A uniform distribution from 0 to 0.6 ml/g was assigned for the waste package corrosion products (BSC 2004e, Table 8.2-2).

The DOE Peak Dose Model used a long-term weighted average for determining the infiltration rates from 10,000 to 1 million years. High, medium, and low rates were obtained by averaging the infiltration rates for each climate state expected to occur during that time frame (OCRWM 2005, Table 1). The probabilities for high, medium and low infiltration rates are 35%, 41%, and

24%, respectively. Since this approach did not include the period from 0 to 10,000 years, it was necessary to revise the DOE Peak Dose Model to include this period. This was done using infiltration rates from Table 2 of OCRWM 2005 for present-day (0 to 600 years), monsoon (600 to 2,000 years), and glacial-transition (2,000 to 10,000 years) climates.⁷ These infiltration histories are shown in Figure 2. Note that the plateaus on the right in this figure extend to 1 million years.

In summary, changes from the DOE Peak Dose Model to create the EPA Uncertainty Model included the following steps:

- Removal of drip shields from system
- Assumption that early waste package failures occurred uniformly from 0 to 5,000 years
- Changing the time steps used in the early period (0 to 5,000 years) from 5,000 years to 500 years per step
- Addition of Tc-99 and I-129 to the suite of radionuclides
- Addition of 0 to 10,000-year infiltration rates
- Remediation of minor programming errors (see Appendix A)

A brief listing of the changes required to create the EPA Uncertainty Model is provided in Appendix A to this report. A complete list of all model changes is included in an Excel spreadsheet (*ModificationLog.xls*). This large spreadsheet is not included here, but is part of the Quality Assurance Program. Additional details on Quality Assurance activities are included in a separate report.

The two modes of operation of the EPA Uncertainty Model are compared with the DOE Peak Dose Model *base case* in Figure 3. The overlap of the two plots with no early failures indicates that the addition of Tc-99 and I-129 to the DOE Peak Dose Model (with waste package failures due only to general corrosion) results in negligible change to the mean peak dose of 125 mrem/yr at 730,000 years. The peak dose using the EPA Uncertainty Model in the early failure mode is 342 mrem/yr at 60,000 years, with a large portion of the dose due to Pu-239. As will be discussed in Section 3.2, the early peak in Figure 3 is based on the assumption that 520 waste packages fail prior to 5,000 years.

⁷ The EPA Uncertainty Model uses 500-year time steps from 0 to 5,000 years, 1,000-year time steps from 5,000 to 10,000 years, and 2000-year time steps from 10,000 years to 50,000 years. As a result, the present-day climate conditions occur from 0 to 1,000 years and the monsoon climate 1,000 to 2,500 years. The glacial-transition climate state occurs from 2,500 to 12,000 years.

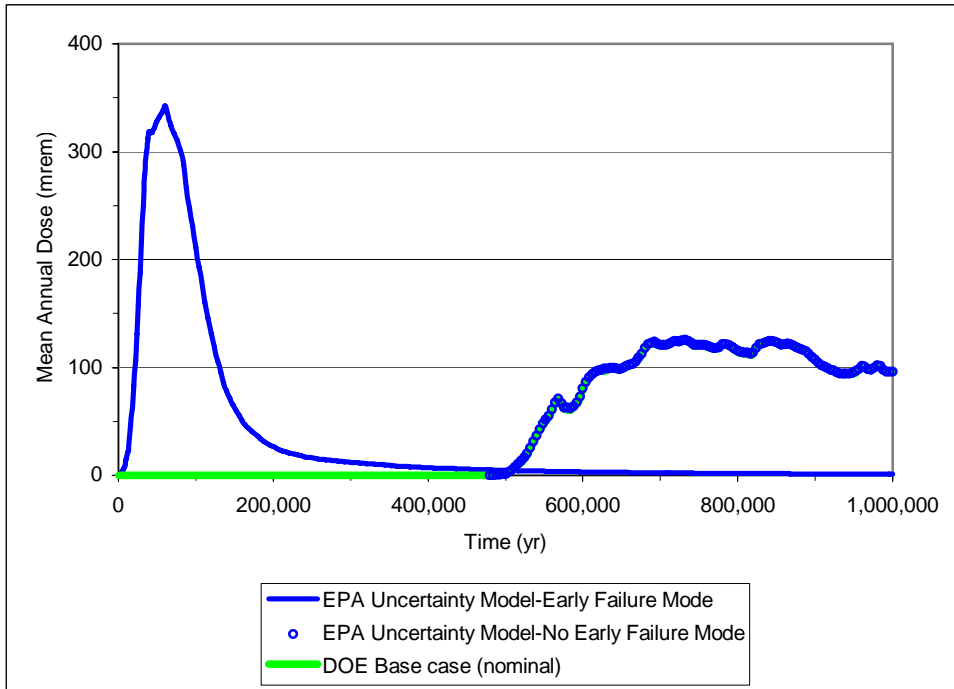


Figure 3. Annual Dose Forecasts for Two Modes of the EPA Uncertainty Model Compared to the DOE Base Case (Nominal)
 (Plots are means of 1,000 realizations.)
 (Source: Runs 1, 10, and 17)

With the changes noted above, the EPA Uncertainty Model retains the capability to model waste package failure by general corrosion, and has the additional capability of determining the doses that may result from early waste package failures. The early failure mode is necessary to examine the evolution of a hypothetical disposal facility at the Yucca Mountain site that is at the “edge of compliance” out to the time of peak dose. To characterize this hypothetical facility, it is necessary to determine the number of failed waste packages that would result in a mean dose of 15 mrem/yr at 10,000 years. At this step in the process, it was necessary to specify the model more precisely to determine the fixed number of early failures. It was decided that the dose estimate would be based on the mean of 1,000 model realizations with all parameters treated stochastically, varying over ranges specified in the *base case* of the DOE Peak Dose Model. The results of this calculation, and additional details on the sensitivity to the selected number of realizations, are presented and discussed further below.

The fully stochastic calculation gives results that answer the question of what peak doses can arise from a hypothetical disposal system at Yucca Mountain that is at the edge of compliance, i.e., gives a mean dose of 15 mrem/yr at 10,000 years. However this result is essentially a "black box" calculation without additional insight concerning the role of individual "driver" parameters in the fully stochastic calculations. For sensitivity studies examining the effects of variations in the major "driver" parameters, all variable parameters in the model are set to their mean values, while the parameters of interest are varied across their expected range. The general approach to the driver parameter sensitivity analyses included these steps:

- (1) Using the fixed number of waste package early failures, develop the deterministic EPA Baseline with all parameters set at their mean values.
- (2) Analyze the sensitivity of doses to the RMEI by varying selected parameters or parameter groups over the assigned uncertainty/variability ranges, while holding all other parameters at the EPA Baseline (mean) values. Sensitivity studies included changes in infiltration rate, seepage-related factors, radionuclide solubilities, and others, both separately and in combination. Section 4 describes the results of the sensitivity studies in detail.

To perform these calculations, it was necessary to search the DOE Peak Dose Model for all variable or stochastic parameters. The DOE Peak Dose Model contains 102 stochastic parameters; however, 3 of these have discrete distributions with categorical outcomes that function as control switches. The control switches are (1) *Infiltration_Case_S*, (2) *Cracks_Before_Patches*, and (3) *Starting_Water_Chemistry*. Of these, only *Infiltration_Case_S* has a significant effect in the model. The control for this variable was manually adjusted in the sensitivity analyses. The remaining 99 distributions include a variety of parameters. Some are used only in the seismic and igneous scenarios, which are not considered in the EPA Uncertainty Model. All other parameters were set to their mean values for the EPA Baseline.

The sensitivity analysis required holding some parameters at their mean, while others are permitted to vary. Since GoldSim does not directly have the ability to control individual variables in this way, EPA developed an Excel spreadsheet that operates in GoldSim and returns the statistic of interest. The spreadsheet *SelectValue.xls* is linked to each GoldSim stochastic element, accepting a GoldSim distribution as input, and returning a value for that parameter as an output in each realization of the model. The spreadsheet allows the user to investigate and control the model in novel ways, such as running the model with all variable parameters in their 40th to 60th percentile range; or all values within the mean +/- one standard deviation; or all values equal to their mean. In addition, the spreadsheet allows for individual variables to be turned on and off, making it possible to study the sensitivity of individual variables. Only two of the available options were used in this study; the spreadsheet returns either a mean value or the original GoldSim stochastic value.

To provide the reader with the proper context for understanding the subsequent sections describing the dose results obtained with the EPA Uncertainty Model, the following key points about the model are reiterated:

- The EPA Uncertainty Model is based on the DOE Peak Dose Model. All model parameters with their associated uncertainties are taken from the DOE Peak Dose Model or from other relevant AMRs prepared by DOE as part of the Yucca Mountain Project.
- The model describes a hypothetical geologic repository designed to generate a mean dose to the RMEI of 15 mrem/yr at 10,000 years. This is termed a repository operating at the “edge-of-compliance.”
- In order to analyze the performance of the natural barrier system of the repository, the influence of the EBS is removed.

- A small, fixed number of waste packages, sufficient to produce the desired dose at 10,000 years, are allowed to fail. No additional waste package failures are assumed to occur, since the focus of the modeling effort is on long-term performance of the natural barriers for a system at the edge-of-compliance.
- Modifications are introduced into the model to address the fact the DOE Peak Dose Model did not consider times less than 10,000 years.
- The time at which the peak dose occurs in the EPA Uncertainty Model has no specific relevance to the Yucca Mountain repository, since only a limited number of waste packages are assumed to fail in the EPA model.

3.2 EPA UNCERTAINTY MODEL – BASELINE ESTIMATES

The number of waste packages that must fail to achieve a mean annual dose of 15 mrem/yr at 10,000 years was determined iteratively. The revised model was first run under the assumption that all waste packages ($N_0=11,184$) would fail at times that are uniformly distributed between 0 and 5,000 years. The mean annual dose at 10,000 years for this run was recorded as D_0 mrem/yr. A fraction equal to 15 mrem/yr divided by the recorded dose was determined; $f_1 = 15/D_0$. The number of waste packages designated to fail in the next run of the model was $N_1 = f_1 N_0$. A mean annual dose of approximately 15 mrem/yr at 10,000 years was generated after several iterations of the procedure, where $N_j = f_j N_{j-1}$, and $f_j = 15/D_{j-1}$.

The DOE Peak Dose Model maintains separate inventories for commercial spent nuclear fuel (CSNF) and codisposal (CDSP) waste packages. The procedure defined above required several iterations, because the number of failed CSNF and CDSP waste packages must be specified separately, and each number must be an integer. The percentage of CSNF waste packages selected for early failure is 69.5% at each stage of the procedure, as in the original DOE Peak Dose Model, to within rounding error due to the discrete counts. It was determined that failure of 520 waste packages at times uniformly distributed between 0 and 5,000 years would generate a mean annual dose forecast of approximately 15 mrem/yr at 10,000 years. This number includes 362 CSNF and 158 CDSP waste packages.

The analyses presented here are essentially comparative in nature, in that a hypothetical disposal system was created using the DOE model, with its built-in conservatisms and then the peak dose projections made relative to that hypothetical starting point. In essence, the conservatisms in estimating releases counterbalance each other. A less conservative model would require more waste packages to be failed to produce the 15 mrem/yr dose at 10,000 years, making more radionuclides available for release in the longer term to contribute to the peak dose. It is not possible to quantitatively assess the relative effects of conservative assumptions on these analyses without a more complex site model. Since the analyses presented here are comparative, the inherent conservatisms in the DOE model should not bias the results, as long as there are no changes in the model structure and assumptions between the calculations used to set up the 10,000-year “edge-of-compliance” disposal system and the calculations to assess its range of peak dose estimates.

Dose versus time results based on 1,000 realizations of the EPA Uncertainty Model are shown in Figure 4. The figure shows plots of the mean and median annual dose as a function of time. The 5th, 25th, 75th, and 95th percentiles are also shown, along with the upper and lower bounds. Figure 4 and all subsequent figures generated by the EPA Uncertainty Model in the early failure mode include only the dose due to the 520 early waste package failures, not the full complement of 11,184 waste packages scheduled for disposal in the Yucca Mountain repository. In this sense, the calculations may underestimate the “actual” dose in that no additional failures are allowed. However, this exercise is focused only on how uncertainties affect the range of dose estimates for the reference case -the hypothetical disposal system at Yucca Mountain at the “edge of compliance” at 10,000 years, rather than an exercise to examine the expected performance of the actual disposal system. This latter objective is the focus of the regulatory compliance decision to be made by the Nuclear Regulatory Commission upon examination of DOE's projections of actual repository performance.

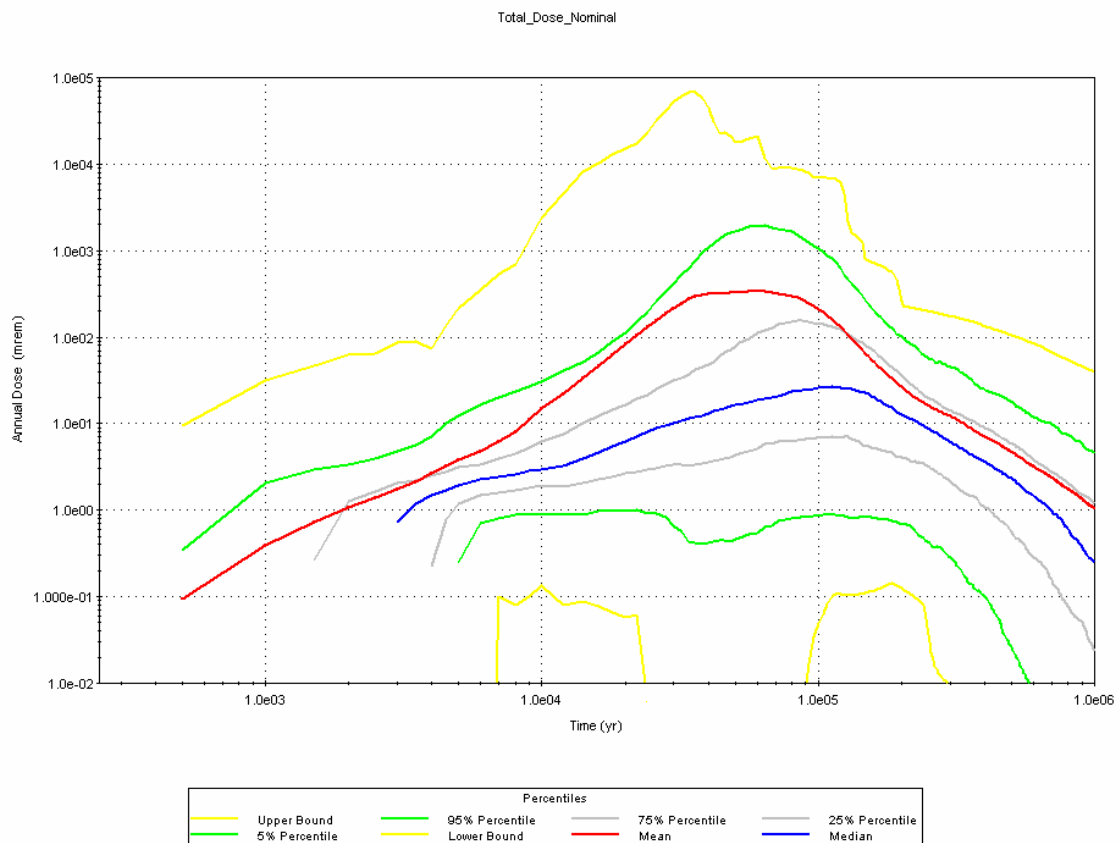


Figure 4. Total Annual Dose, Mean and Selected Percentiles of 1,000 Realizations for EPA Uncertainty Model
(Source: Run 1)

The mean annual dose from early failures in Figure 4 is 15 mrem/yr at 10,000 years, and the mean annual dose reaches a peak of 342 mrem/yr at 60,000 years based on 1,000 realizations of the model. The median annual dose at 10,000 years is 3 mrem/yr, and the median annual dose reaches a peak of 27 mrem/yr at 112,000 years. These results also provide some important insight about the increase in uncertainty in long-term performance projections for the Yucca

Mountain disposal system. By comparing the difference between the 5th and 95th percentile curves in this figure, it can be seen that uncertainty, as measured by the difference between the two curves, generally increases over time up to the time of the peak dose, at which point the spread in the dose is over 3 orders of magnitude (ranging from less than 1 mrem/yr to over 1 rem/yr.). The spread (uncertainty) at 10,000 years is about 1.5 orders of magnitude. Beyond the time of the mean peak dose at 60,000 years, uncertainties decrease with time to about two orders of magnitude at 200,000 years and then begin to increase again, reaching a value of 4.6 orders of magnitude at 1 million years. The 5th percentile values remain reasonably constant to about 200,000 years and then begin to decline, while the 95th percentile values increase to the time of the peak dose and then begin to decline. The rate of decline of the 5th percentile values after about 200,000 years is more rapid than for the 95th percentile values, causing the ratio to increase for times between 200,000 and 1 million years. This behavior may be driven by the changing role of the various radionuclides with time as will be discussed subsequently.

These results provide an answer to the primary objective of the assessments—to examine the consequences of uncertainties, in the characteristics and functions of the disposal system, on very long-term dose projections for the site. Results of these calculations show that uncertainties over the very long-term are manifested in generally increasing spread of dose projections over time. Further insight on the propagation of uncertainties can be gained by examining the results of sensitivity studies described in Section 4. Examining the various plots of projected doses for the sensitivity analyses shows that the spread between the 5% and 95% values increases through the period of peak dose.

There is a distinct dip in the lower bound and 5th percentile at the time of the peak mean dose in Figure 4 that is traceable to the behavior of individual realizations. Realizations with double peaks are common. A "deep valley" pattern occurs in a small fraction of these realizations. The valley at 60,000 years is presumed to be due to complete removal of Tc-99 before that time. Eventually, other slower-moving species reach the receptor location, creating a second peak in the total dose. In general, the double top pattern is due to the separation of the fast- and slow-moving species, given the finite masses in the source term.

The EPA Uncertainty Model conducts a Monte Carlo simulation to assess the range of uncertainty in annual dose forecasts due to variations in the stochastic parameters used by the model. A larger number of realizations generally implies a more stable forecast, however a trade-off exists between the greater precision offered by higher sample sizes and the time required to generate the desired number of realizations. The results presented in this report are based on a sample of n=1,000 realizations, the same number used in the DOE Peak Dose Sensitivity Analysis. The EPA Uncertainty Model takes approximately 100 minutes to generate 1,000 realizations.

Results of the simulations will change if more or less than 1,000 realizations are included. The sensitivity to the number of realizations introduces another source of variability in the model results. An analysis was conducted to assess the sensitivity of the forecasted peak mean and median annual doses to a change in the number of realizations. A wide range of sample sizes was examined; n=300, 500, 1,000, 1,500, 2,000, 2,500, 3,000, 4,000, and 5,000. The same initial

seed value⁸ was used in all simulations; hence each run includes all realizations in any run with a smaller sample size plus an additional number of newly generated realizations. For example, the run with 1,500 realizations includes all realizations in the size-1,000 run, plus an additional 500 newly generated realizations.

The forecasted mean and median annual doses at 10,000 years and at the time of the peak mean or median annual dose are shown in Table 1 for each size sample. The shading in row *c* indicates the EPA Baseline with 1,000 realizations. Also shown in parentheses in this row are the upper and lower bounds of the 95% confidence interval for the estimated mean at 10,000 years and at the time of the peak mean dose, based on 1,000 realizations. Note that these confidence intervals include the forecasted doses based on all runs with higher sample sizes. A plot of the peak mean dose for each sample size is shown in Figure 5. Also shown in the figure are the upper and lower bounds of the 95% confidence interval for the mean based on 1,000 realizations. The forecasted values of the peak mean dose range from 328 to 397 mrem/yr. All forecasted peak mean doses fall within the 95% confidence interval for the mean, based on 1,000 realizations. A plot of the peak median dose for each sample size is shown in Figure 6. Estimates of the peak median dose are much more stable than the forecasts of the peak mean dose, with a range from 25.4 to 33.1 mrem/yr.

Two additional model runs were made to determine the effect of changing the initial seed from its default value of 1. Runs of 1,000 and 2,000 realizations were made using 11337 as an arbitrarily selected alternative seed. Results of these runs are reported in the Quality Assurance document that accompanies this report. The run of 1,000 realizations generated a mean dose of 7.53 mrem/yr at 10,000 years (50% lower than the 15 mrem/yr dose at 10,000 years in row *c* in Table 1 with seed = 1), and a peak dose of 353.0 mrem/yr at 60,000 years (3% higher than the peak dose which occurs at the same time in row *c*). The results for 1,000 realizations with the new seed are similar to those in row *a* of Table 1 with 300 realizations, except for the time of the peak dose. As in row *a*, the mean dose at 10,000 years with the new seed falls slightly below the 95% confidence interval for the mean shown in row *c* of Table 1. The peak dose with the new seed falls within the confidence interval for the peak dose shown in row *c*. The run of 2,000 realizations with the new seed generated a mean dose of 8.87 at 10,000 years (approximately 23% lower than the mean dose of 11.5 mrem/yr at this time for row *e* with seed = 1), and a peak dose of 382.1 mrem/yr at 60,000 years (2% lower than the peak dose of 389.9 mrem/yr for row *e*). Both results with the new seed fall within the corresponding 95% confidence intervals shown in row *c*.

All results with the new seed value are within the range of values shown in rows *a* through *i* in Table 1. In general, the runs for 1,000 and 2,000 realizations with the new seed show more agreement than exists between the corresponding runs in rows *c* and *e* in Table 1 with the original default seed. There is greater agreement between the peak doses with different seeds than there is between the doses at 10,000 years with different seeds.

⁸ Simulation models use a non-repeating sequence of random numbers to model the effects of variability and uncertainty in the model parameters. The sequence of random values is determined by selecting an initial (seed) value to begin the sequence for each run of the model. When a different initial seed is used, a different sequence of random numbers is used in that run of the model.

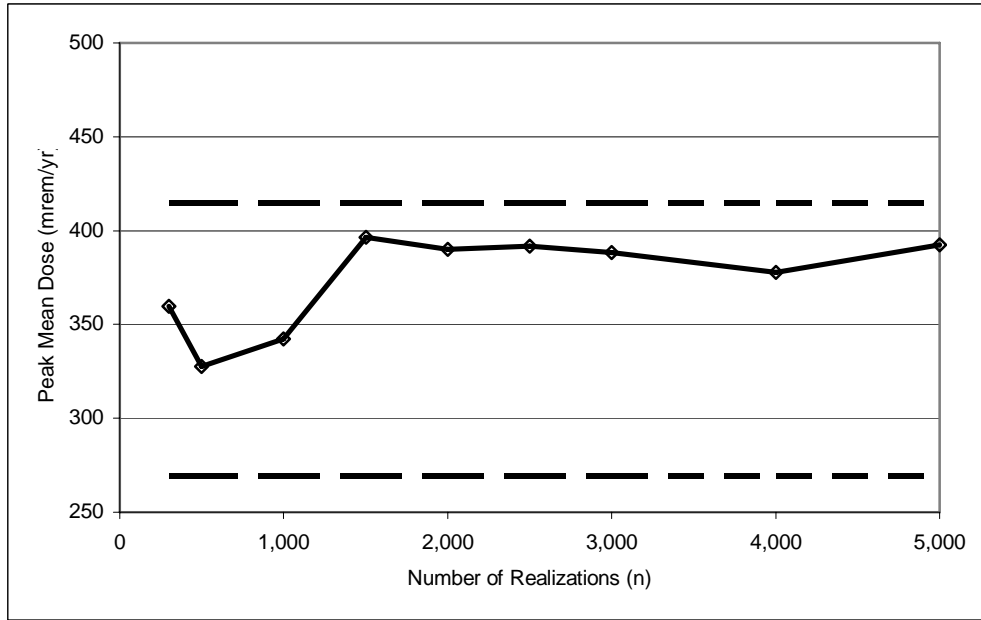


Figure 5. Plot of EPA Uncertainty Model Peak Mean Dose Forecast versus Number of Realizations (n)
 (Dashed lines indicate upper and lower bounds of approximate 95% confidence interval for estimated mean with n=1000.) (Source: Run 11)

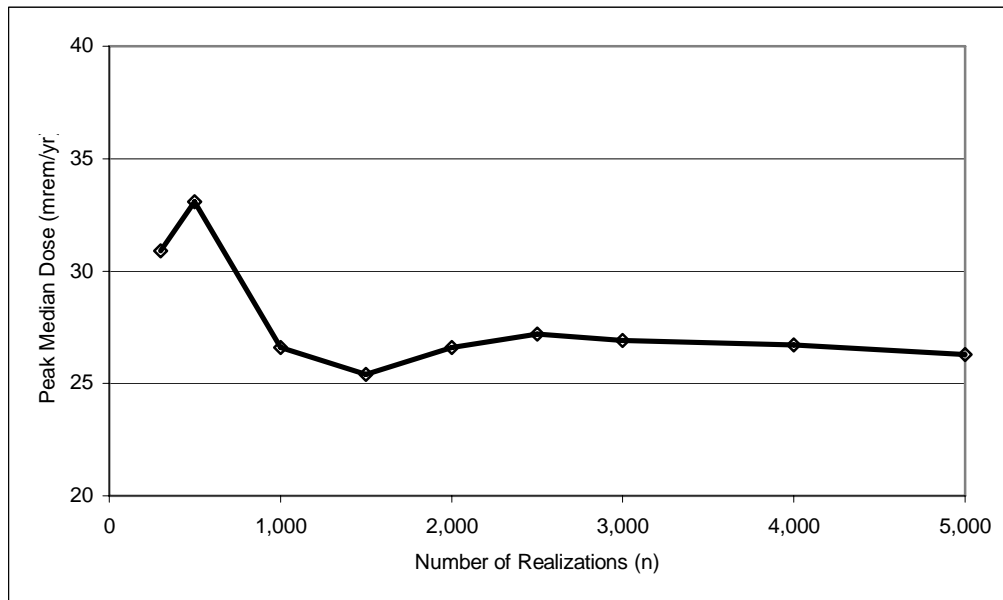


Figure 6. Plot of EPA Uncertainty Model Peak Median Dose Forecast versus Number of Realizations
 (Source: Run 11)

Table 1. EPA Uncertainty Model Mean and Median Annual Dose Forecasts at 10,000 Years and at Peak Dose for up to 5,000 Realizations Using the Same Initial Seed (Seed = 1)
(Source: Run 11)

Number of Realizations	Forecast of Annual Dose at 10,000 Years		Forecast of Peak Annual Dose			
	Mean (mrem/yr)	Median (mrem/yr)	Mean (mrem/yr)	Year ⁽¹⁾	Median (mrem/yr)	Year ⁽¹⁾
a) n=300	7.52	3.03	359.8	52,000	30.9	120,000
b) n=500	7.66	3.11	327.8	56,000	33.1	104,000
c) n=1,000	15.0 (8.5,21.6) ⁽²⁾	2.98	342.2 (269, 415) ⁽²⁾	60,000	26.6	112,000
d) n=1,500	12.4	2.97	396.5	60,000	25.4	112,000
e) n=2,000	11.5	3.00	389.9	60,000	26.6	116,000
f) n=2,500	10.7	3.02	391.8	56,000	27.2	116,000
g) n=3,000	10.2	3.04	388.3	56,000	26.9	116,000
h) n=4,000	9.80	3.06	377.6	52,000	26.7	116,000
i) n=5,000	11.3	3.07	392.5	48,000	26.3	116,000

⁽¹⁾ The model uses 2,000-year time steps from 10,000 to 52,000 years and 4,000-year time steps from 52,000 to 1,000,000 years.

⁽²⁾ An approximate 95% confidence interval for the estimated mean is shown in parentheses for n = 1,000 realizations.

Figure 7 shows the contributions to the mean annual dose by radionuclide. The mean annual dose for early failures is dominated by Pu-239, with Pu-240 being the second most important contributor to doses from early failures. The highly mobile species, Tc-99 and Np-237, are also significant contributors to doses prior to 10,000 years. As noted earlier, doses to the RMEI in the DOE Peak Dose Model *base case* are dominated by Pu-242 and Np-237, with half-lives of 3.75×10^5 and 2.14×10^6 years, respectively. The important nuclides contributing to early failure doses have shorter half-lives (2.41×10^4 years for Pu-239 and 6.56×10^3 years for Pu-240), and have significantly decayed by the time of the peak dose in the DOE *base case* (e.g., about 730,000 years).

To test the behavior of the EPA Uncertainty Model, calculations were made for variations in the length of SZ and infiltration rate using switches built into the DOE Peak Dose Model. Results showing sensitivity to the length of the SZ (alluvium or no alluvium)⁹ and the length of the alluvium combined with a high infiltration rate are presented in Figure 8.

⁹In the base case of the DOE Peak Dose Model, the flow and transport submodel below the EBS does not consider the UZ or the portion of the SZ upstream of the alluvium. Thus, only a portion of the 18-km pathway to the RMEI is included.

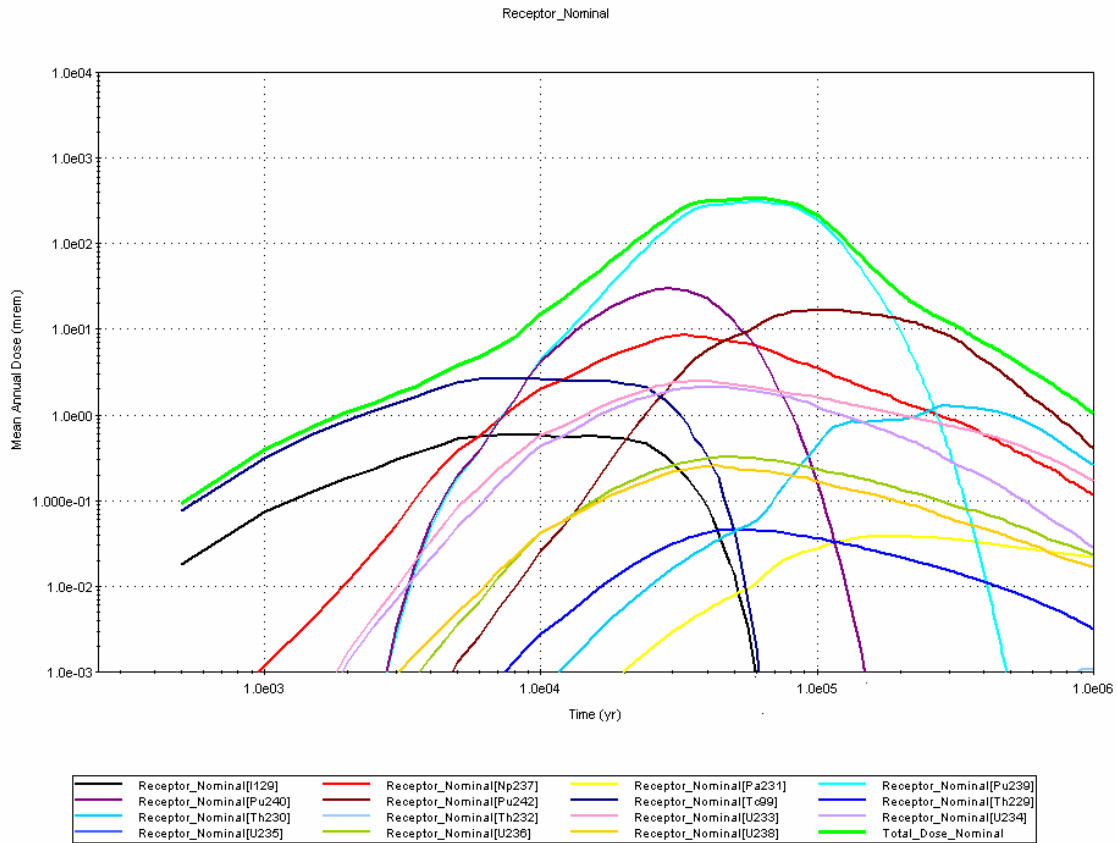


Figure 7. Mean Annual Dose by Radionuclide, 1,000 Realizations of EPA Uncertainty Model
(Source: Run 1)

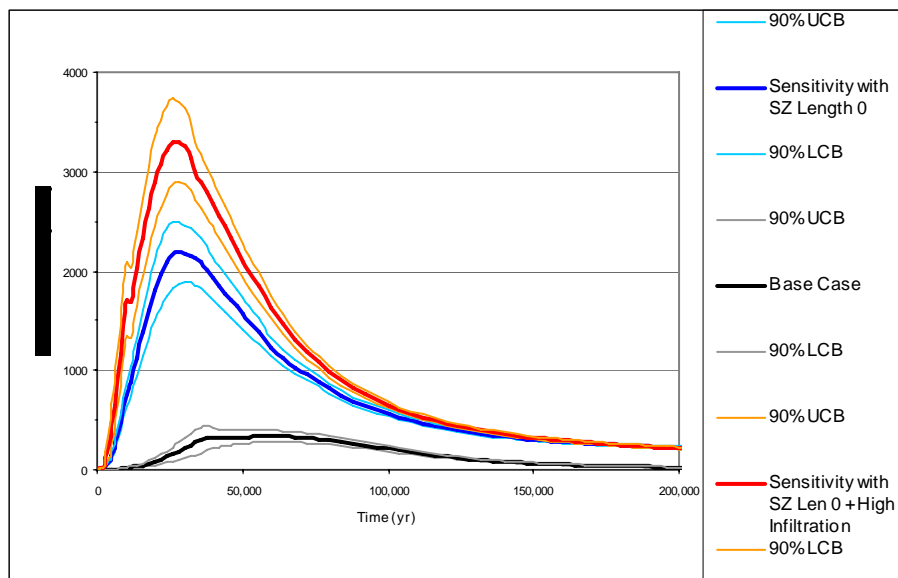


Figure 8. Mean Annual Dose and 90% Confidence Limit
(Base Case, SZ length = zero, and SZ length = zero plus high infiltration.) (Source: Runs 1, 12, and 13)

Output graphs generated by GoldSim usually show the mean realization and percentiles at each point in time for a single run of the model (for example, see Figure 4). In that type of graph, the difference between the 5th and 95th percentiles shows the spread of the 1,000 realizations around their mean value. Figure 8 shows three mean value curves from different runs (Sets of 1,000 realizations). For each mean, the upper and lower 90% confidence bounds (UCB and LCB) for the mean are also shown. The confidence bounds reflect the sampling error that is expected when 1,000 realizations are used to estimate the mean. The sampling error of the mean at each time was estimated by dividing the standard deviation of each set of realizations around their mean by the square root of 1,000. While 1,000 is a relatively large number of realizations, the sampling error for the mean is not negligible, as shown by the spread between the 90% UCB and 90% LCB in Figure 8. These limits denote the upper and lower bounds of a 90% confidence interval for the estimated mean. Note, however, that the confidence intervals are sufficiently narrow to demonstrate that each mean curve is significantly different from the other two.

Figure 8 demonstrates that the reduced length of the SZ and a high infiltration rate significantly increase the mean peak dose, as compared to the *base case*. The standard error of the mean also increases in those scenarios. These results are intuitively correct, and illustrate that the model performs as expected with the changes that were made to the DOE Peak Dose Model configuration and the insertion of the new radionuclides.

The sensitivity of the number of failed waste packages required in the early failure mode to obtain a mean dose of 15 mrem/yr at 10,000 years was assessed by examining a less conservative site model in which the SZ length is increased by a factor of 2. This calculation is designed to show the number of failed waste packages that would be required by a site model, which would approximate additional retardation during transport through the UZ below the repository and in the SZ before reaching the alluvium.¹⁰ The EPA Uncertainty Model was first run for 520 waste package failures, with the SZ length increased by a factor of 2. The results indicated a mean annual dose of 7.12 mrem at 10,000 years. Using this less-conservative site model, 1,079 early waste package failures would have been required to obtain a mean annual dose of 15 mrem at 10,000 years. The early failures include 750 CSNF and 329 CDSP waste packages.

With the increased number of waste package failures, the new site model forecasts a peak mean dose of 365.1 mrem/yr at 46,000 years. This peak is approximately 7% higher than the peak dose forecast from the EPA Uncertainty Model shown in row *c* in Table 1. This low sensitivity demonstrates that the choice of the somewhat conservative DOE Peak Dose Model as a basis for modeling a disposal facility at the “edge-of-compliance” at the Yucca Mountain site is robust with respect to changes in the degree of conservatism reflected in the model. A more realistic site model is likely to generate similar estimates for the peak dose obtained within the period of geologic stability by a facility at the edge of compliance with the 10,000-year standard.

¹⁰ It is recognized that this is only an approximation, since flow mechanisms in the UZ and the fractured volcanics in the SZ are different from the SZ alluvium. However, this sensitivity test does provide a semi-quantitative evaluation of the effects of retardation along an increased flow path.

3.3 EPA BASELINE FOR SENSITIVITY ANALYSES

As mentioned above, the fully stochastic analyses provide the range of peak doses expected for the 10,000-year “edge of compliance” disposal system at peak dose time. To facilitate interpretation of these analyses, a series of sensitivity studies are presented in this report in Section 4. For these analyses, all the variable parameters were set to mean values except the parameter (or parameter group) of interest, which was allowed to vary across the expected range. In order to have a baseline for comparison with the sensitivity studies, the 520 waste packages were fixed to fail at 2,500 years (midway between the 0 and 5,000 year period set for the stochastic analyses), and the other variable parameters were set to their mean values for the 10,000-year period. The EPA Baseline dose was then calculated for comparison with the doses calculated for sensitivity study results.

As noted above, several input parameters are discrete or categorical. These include the following:

- (1) *Cracks_Before_Patches*, a Bernoulli variable with values TRUE or FALSE with probability $p=0.5$: This random variable is used to determine if stress corrosion cracks occur before general corrosion failure. Its outcome determines the pH regime in the failed package in each realization.
- (2) *Starting_Water_Chemistry*, a multinomial discrete choice variable with values 1=HDPERM; 2=CS2000; 3=CS1000; 4=SD-9; 5=CS500 with equal probabilities: This random variable is used to determine which starting water chemistry is applicable for the realization.
- (3) *Infiltration_Case_S*, a multinomial discrete choice variable with values 1=Low, 2=Medium, 3=High with probabilities 0.24, 0.41, and 0.35, respectively: This random variable selects the appropriate infiltration rate used in each realization.

For the EPA Uncertainty Model with fixed parameters, *Cracks_Before_Patches* was set to TRUE by assigning a probability of 0.99999. *Starting_Water_Chemistry* was set to 3, which is equivalent to choosing the median CO₂ partial pressures in Table 6 of the OCRWM 2005. The *Infiltration_Case_S* was set to 2 (Medium). The EPA Baseline annual dose curve is presented in Figure 9. It should be emphasized that this curve is only for the dose from the 520 waste packages with early failures. To obtain a complete picture of the dose history over the period of geologic stability, the dose curve for the long-term failures shown in Figure 3 would be superimposed on this curve beginning around 500,000 years, when general corrosion failure of the waste packages commences.

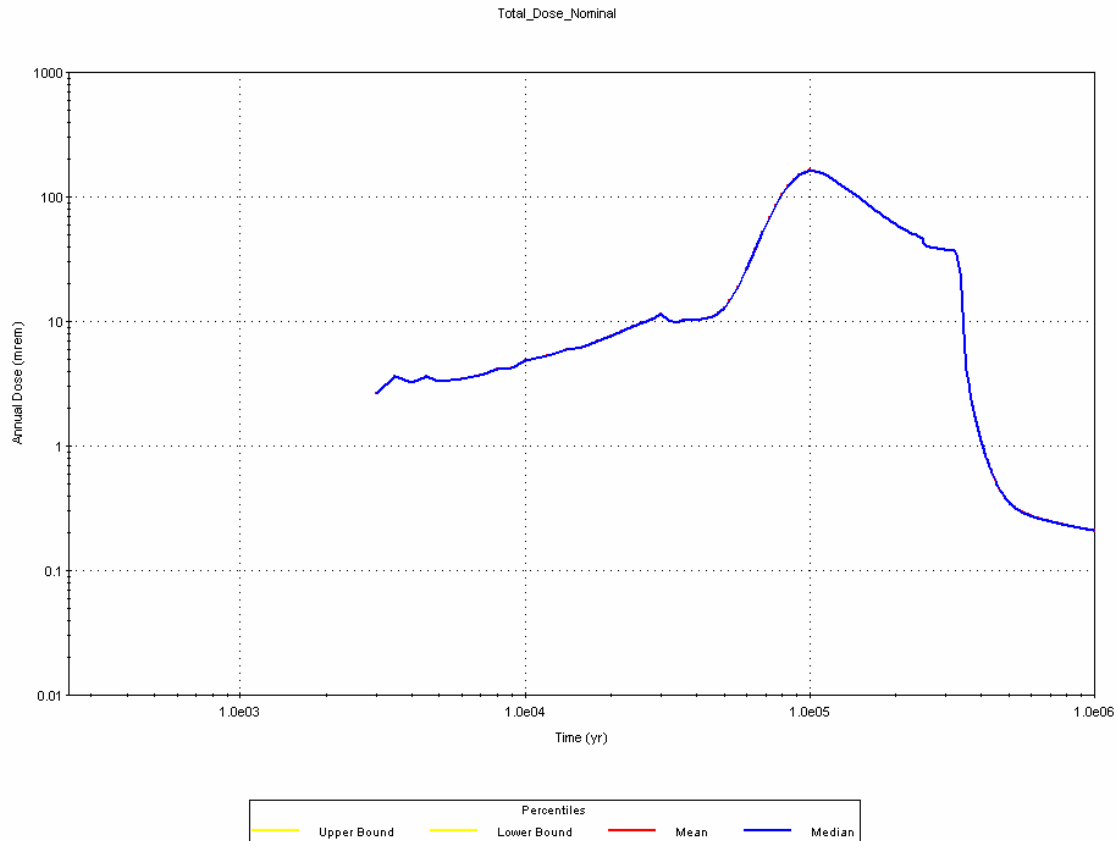


Figure 9. EPA Baseline – Total Annual Dose for 520 Failed Waste Packages with Parameters Fixed at Mean (Infiltration case = 2 (Medium))
 (Annual dose at 10,000 years is 4.8 mrem/yr, and annual dose reaches peak of 163 mrem/yr at 100,000 years.)
 (Source: Run 2)

Although 520 early waste package failures would result in a dose of 15 mrem/yr at 10,000 years when all parameters are allowed to vary over their assigned distributions, the dose at 10,000 years is 4.8 mrem/yr from 520 failed waste packages when all parameters are set at their mean values. In the EPA Uncertainty Model, certain combinations of parameter values, such as high infiltration combined with high solubility, lead to realizations with very high doses. The mean calculated from 1,000 such realizations is significantly influenced by these extreme values. When all parameters are fixed at their means, such extreme combinations do not occur. Hence, the mean of 1,000 realizations is usually greater than the single realization obtained when all parameters are fixed at the mean.

When the EPA Uncertainty Model Baseline is run with all parameters fixed at their mean values, the time of waste package failure also is fixed at its mean value of 2,500 years. The EPA Baseline consists of a single realization, since all parameters are fixed. Alternatively, the time of waste package failure may be permitted to vary over its assigned distribution, which is uniform from 0 years to 5,000 years. A test was performed to determine if the mean of 1,000 realizations with random waste package failure times closely approximates the EPA Baseline shown in Figure 9. The test also examined the effect of a fixed early failure time when all parameters are random, as in Figure 4.

Comparative forecasts of the mean and median annual dose are shown in Table 2 at 10,000 years and at the time of peak mean dose. The five runs compared in Table 2 are *a*) a fixed parameter model with fixed early failure time; *b*) a fixed parameter model with random early failure times; *c*) a random parameter model with fixed early failure time; *d*) a random parameter model with random early failure times; and *e*) a random parameter model with random early failure times but without the LHS sampling option (discussed below). Note that the model highlighted in row *d* of Table 2 is identical to the run in row *c* of Table 1.

Table 2. Mean and Median Annual Dose Forecasts at 10,000 Years and at Year of Peak Mean Dose (mrem/yr)
(Source: Runs 1, 2, 15, 16 and 21)

Model Specification	Forecast of Annual Dose at 10,000 Years		Forecast of Peak Annual Dose	
	Mean	Median	Mean	Median
<i>a</i>) Fixed Parameters with fixed WP failure time (n=1)	4.83	4.83	162.83 @100,000 yr	162.83 @100,000 yr
<i>b</i>) Fixed Parameters with Random WP failure times (n=1000)	4.79	4.78	162.65 @100,000 yr	162.83 @100,000 yr
<i>c</i>) Random Parameters with Fixed WP failure time (n=1000)	14.7	3.03	341.24 @60,000 yr	26.78 @112,000 yr
<i>d</i>) Random Parameters with Random WP failure times (n=1000)	15.0 (8.5, 21.6) ⁽¹⁾	2.98	342.20 (269, 415) ⁽¹⁾ @60,000 yr	26.59 @112,000 yr
<i>e</i>) All Random Parameters with no LHS Sampling (n=1000)	19.7	3.17	408.14 @52,000 yr	31.12 @116,000 yr

⁽¹⁾ The 95% confidence interval for the estimated mean is shown in parentheses.

The mean annual dose at 10,000 years in the EPA Baseline (row *a* with failures fixed at 2,500 years) is 4.83 mrem/yr. The mean annual dose at 10,000 years for the 1000 realizations in row *b* with random failure times is approximately the same at 4.79 mrem/yr. The peak mean dose is reached at 100,000 years in both fixed parameter model runs. At that time, the forecast from the EPA Baseline run is 162.83 mrem/yr, while the peak mean dose with random failure times is essentially the same; 162.65 mrem/yr. At 100,000 years, the median forecast with random failure times is the same.

When the parameters are random but the failure time is fixed in row *c*, the mean dose at 10,000 years is 14.7 mrem/yr. The EPA Uncertainty Model with all parameters random, including the failure time, has a slightly higher mean of 15 mrem/yr at this time. The peak mean doses at 60,000 years differ by less than 1 mrem/yr for runs in rows *c* and *d*, while the medians are almost identical. This demonstrates that the model output is insensitive to the assumption that waste package failures are fixed at 2,500 years, rather than at random times over the first 5,000 years, for both fixed and random parameter models.

One additional model run was also conducted. GoldSim provides an option to use Latin Hypercube Sampling (LHS) when parameter values are selected for each realization. This option is selected in the DOE Peak Dose Model, because it provides an efficient method for estimating the mean annual dose. LHS reduces the variability of the sampling due to its tightly stratified design. The run in row *e* with 1,000 realizations is equivalent to the run in row *d*, except the LHS option was turned off. The forecasted mean dose in this run is 19.7 mrem/yr at 10,000 years, and a peak mean dose of 408 mrem is reached at 52,000 years. The forecasted peak mean dose without the LHS option is higher than the other four model runs shown in Table 2, all nine runs shown in Table 1, and the two runs with an alternative initial seed discussed in Section 3.2. However, the peak mean dose in row *e* lies inside the upper end of the 95% confidence interval of 269 to 415 mrem/yr obtained in row *d* using the LHS option.

4.0 EPA SENSITIVITY STUDIES

This section describes how doses to the RMEI vary over the period of geologic stability when the number of early waste package failures is fixed at 520 and all parameters are fixed at their mean values, except for selected parameters whose sensitivity is being tested. In essence, the sensitivity studies follow the performance beyond 10,000 years of a system that just meets a mean dose criterion of 15 mrem/yr at 10,000 years. Contributions to dose from later-stage general corrosion failures are excluded (i.e., the radionuclide inventory in the repository source term is limited to these failed waste packages whose failure lead to the mean 15 mrem/yr. dose at 10,000 yrs.). The results of the sensitivity tests for specific parameters are then compared to the results of a simulation where all parameters are allowed to vary over their assigned ranges except for the number of failed waste packages, which remains fixed at 520.

4.1 SENSITIVITY TO INFILTRATION RATE

The sensitivity to infiltration rate was examined by replacing the medium infiltration rate used in the EPA Baseline with the high infiltration rate and the low infiltration rate histories presented earlier in Figure 2. All other parameters were held at their mean values. Table 3 compares the results of the three infiltration models.

Table 3. Effects of Infiltration Rates on Dose to the RMEI from Early Waste Package Failures

(Source: Runs 2, 3, and 4)

Infiltration Rate	Dose at 10,000 yr (mrem/yr)	Peak Dose (mrem/yr)	Time of Peak Dose (years)
High	6.4	273	88,000
Medium (EPA Baseline)	4.8	163	100,000
Low	3.5	20	144,000

It is clear that increasing the infiltration rate increases the peak dose and causes the peak dose to occur at earlier times. The peak dose at the high infiltration rate is more than 10-times higher than at the low infiltration rate. The time at which the peak dose occurs has no absolute significance in the EPA Uncertainty Model, since the EPA Baseline is derived from a hypothetical case where a limited fixed number of waste packages fail at a fixed time. However, changes in the time of the peak dose may be useful in comparing sensitivity study results.

As discussed in Section 2.3.1, DOE analyzed infiltration rate sensitivity when the model is run under nominal (*base case*) conditions with fully random parameters (OCRWM 2005, Section 6.4.1). The EPA Uncertainty Model was run under similar conditions to compare the sensitivity to infiltration rates in the two models. Runs (using 1,000 realizations each) were made for the low, medium, and high infiltration scenarios allowing all other parameters to be random (Runs 18, 19 and 20, respectively). The low infiltration case peak dose was 70% lower and the high infiltration case peak dose was 43% higher than the medium infiltration case for these three runs.

DOE reports that the low infiltration case was 35% lower in the peak mean dose, and the high infiltration case was 29% higher than their *base case*, where the infiltration rate was variable. To construct a similar comparison, Runs 18 and 20 were then compared to the EPA Uncertainty Model results with all parameters, including infiltration, varying randomly (Run 1). The low infiltration peak mean dose was 69% lower and the high infiltration peak dose was 50% higher than the EPA Uncertainty Model with random parameters. The EPA Uncertainty Model runs show more dramatic differences than did the DOE Peak Dose Model, in which peak doses occur much farther out in time, i.e., beyond 400,000 years. The increased sensitivity to infiltration in the EPA Uncertainty Model is likely due to the addition of I-129 and Tc-99 that are not contained by the natural barriers.

4.2 SENSITIVITY TO SEEPAGE PARAMETERS

The DOE peak dose sensitivity modeling (OCRWM 2005) showed seepage (ground water that enters the emplacement drifts) to be the major driver for performance; not an unexpected result, since performance is directly a factor of how much water can get to the packages and the wastes. To evaluate the sensitivity of the EPA Baseline to seepage parameters, the seepage parameters from the DOE Peak Dose Model were allowed to vary over their full range of variability/uncertainty, while all other parameters in the EPA Uncertainty Model were held at their mean values. Results of this evaluation are summarized in Figure 10.

From this figure it can be seen that the mean peak dose of 183 mrem/yr occurs at 92,000 years, which may be compared to the peak dose for the EPA Baseline with a dose of 163 mrem/yr at 100,000 years (see Figure 9). By adding seepage parameter uncertainty and variability to the EPA Baseline, the spread in the total dose between the 5th and 95th percentiles is approximately 3 mrem/yr at 10,000 years, and this spread increases to 482 mrem/yr at the time when the 95th percentile dose reaches its peak value. It should be noted that this level of uncertainty is associated with the medium infiltration rate scenario, which is the scenario included in the EPA Baseline.

Another measure of the sensitivity of dose to the RMEI from seepage can be made by comparing the results of the case where drift collapse is included in the model (as it is in the DOE Peak Dose Model *base case* and the EPA Uncertainty Model) with the case where drifts are not collapsed (a sensitivity option included in the DOE Peak Dose Model). Differences between the collapsed and non-collapsed models include the following:

- Use of an 11-m collapsed drift diameter¹¹ versus a 5.5-m diameter for intact drifts doubles the amount of percolation flux, thereby increasing seepage rates
- Use of substantially different response surfaces for seepage fraction and seepage flow rates (OCRWM 2005, Appendix A)

¹¹ A large number of drift collapse scenarios were considered by DOE. This is the largest drift diameter after collapse (BSC 2004, p. 6-29).

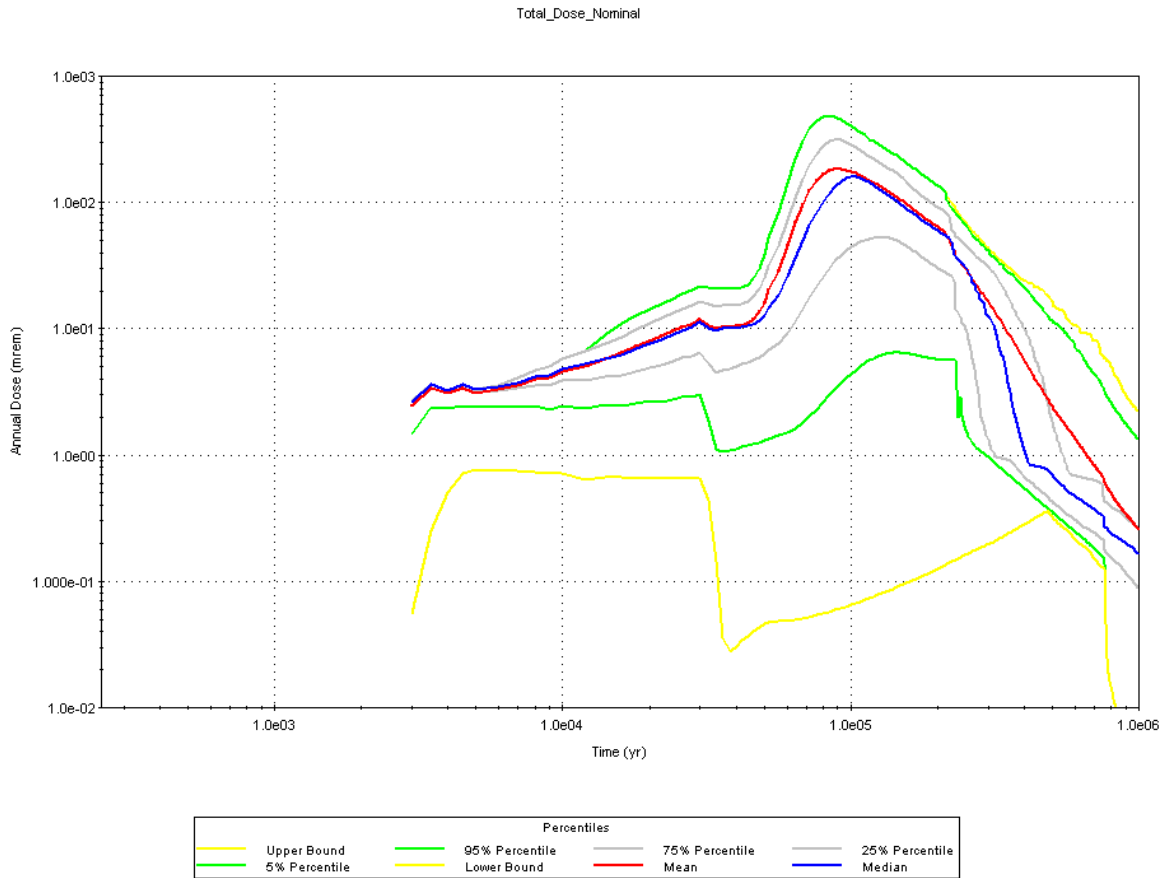


Figure 10. Mean and Selected Percentiles Showing Sensitivity of Total Annual Dose to Seepage Parameters in EPA Uncertainty Model

(Sensitivity analysis using Uncertainty Model with all parameters at mean except for four seepage parameters: *k_lith*, *k_nonlith*, *one_over_alpha_A*, and *Flow_Focusing_Factor*. 520 WPs with early failure at 2,500 yr, 1000 realizations, Infiltration case=2 (Medium).) (Source: Run 5)

Seismic events are a potential source of energy, which could cause drift collapse. According to BSC 2004, seismic-induced peak ground motions in excess of 2 m/s can cause collapse of emplacement drifts in lithophysal rock units. It can be deduced from Table 16 of OCRWM 2005 that the exceedance frequency for this peak ground velocity is about $2 \times 10^{-6}/\text{yr}$. However, in non-lithophysal units, only minor damage from wedge-type rockfalls occurs from all seismic events. About 15% of the drifts are in non-lithophysal rocks, where drift collapse will not occur, and 85% are in lithophysal rocks, where the exceedance frequency for drift collapse is no greater than $2 \times 10^{-6}/\text{yr}$. Thus, over 1,000,000 years, two seismic events capable of inducing drift collapse are expected to occur. There is a 1-in-5 chance of such an event occurring in the first 100,000 years, and a 1-in-50 chance of such an event occurring in the first 10,000 years. Clearly, the assumption that drifts have collapsed and cause increased seepage is conservative, when evaluating the impacts of early waste package failures.

Results for the non-collapsed drift case with all parameters set at the mean (including a medium infiltration rate) are shown in Figure 11. The total annual dose at 10,000 years is 1.5 mrem/yr, and the total annual dose reaches a peak of 1.9 mrem/yr at 700,000 years.

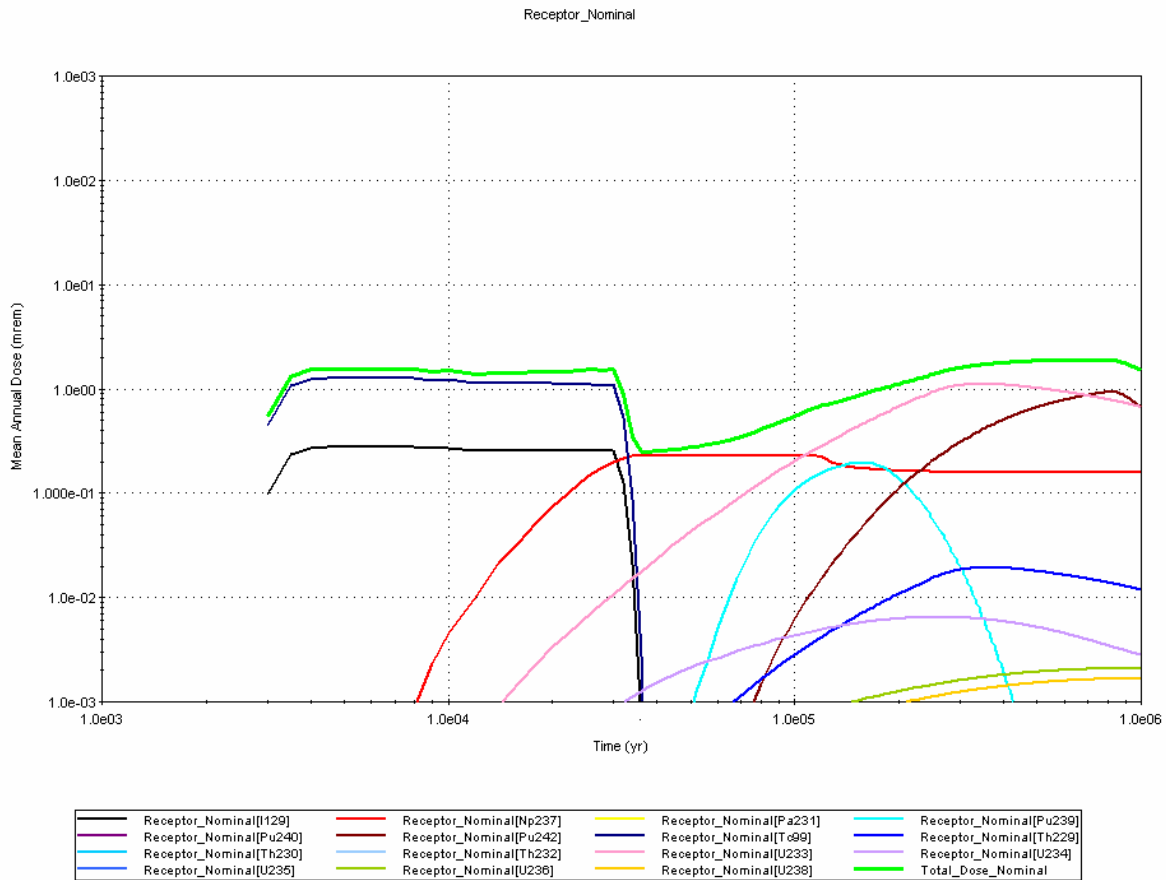


Figure 11. Mean Annual Dose by Radionuclide for EPA Baseline with Non-Collapsed Drift Conditions
(Source: Run 9)

A dramatic difference exists for the collapsed drift case. The EPA Baseline has a peak dose from early failures of 163 mrem/yr at 100,000 years (Figure 9), while the EPA Baseline modified for seepage associated with non-collapsed drifts (Figure 11) reaches a peak dose of only 1.9 mrem/yr at 700,000 years. All parameters are fixed in both Figures 9 and 11. (The dose-versus-time curve also has an earlier peak of 1.6 mrem/yr at 30,000 years.) The difference is due to the wide differences in the response surfaces for the collapsed and non-collapsed drift seepages when *one_over_alpha_A*, *k_lith* and *k_nonlith* parameters are set to their mean values, as shown in Appendix A of OCRWM 2005.

4.2.1 Regression Analyses of Seepage Parameters

Regression analysis was used to determine which model parameters have the largest influence on the peak dose. Software included in the Statistical Package for the Social Sciences (SPSS) was used to run the regressions. This package of statistical programs has a long history of use in the social sciences and health professions, dating back to the mainframe era. It now is available

commercially in Windows.¹² The SPSS stepwise regression procedure was used to determine the relative importance of the four seepage parameters in terms of their contribution to the variation in forecasted annual dose shown in Figure 10. The four seepage parameters for this analysis are shown in Table 4. The table shows the name, description, location in the GoldSim model, and the distribution assigned for each seepage parameter.

Two of the seepage parameters, k_{lith} and $k_{nonlith}$, are assigned distributions based on the logarithm of k . The data for the stepwise analysis consist of the (logged) peak dose forecast and the four seepage parameter values used for the 1,000 realizations from Run 5. GoldSim selects one set of values for the stochastic parameters in the model at the start of each realization and uses these values for all time steps in that realization. A new set of parameter values is then selected for the next realization.

The dependent variable for the stepwise regression procedure is the base-10 logarithm of the peak dose reached over the 1,000,000-year time period spanned by the EPA Uncertainty Model runs. The peak dose forecasts from this sensitivity run (Run 5) were obtained by fixing all parameters other than the four sensitivity parameters at their mean value. In a few realizations, the observed peak dose occurs at 1,000,000 years. Since some containers always fail in the early failure period, there are no realizations with a zero peak dose.

The four seepage parameters are the four explanatory variables in the regression, which also includes a constant term. Unless otherwise directed, GoldSim treats all stochastic parameters as independent random variables. This avoids any possible problems in the interpretation of regression results due to collinearity between the explanatory variables.

The regression procedure selects, in stepwise order, the parameters that best explain the variation in the peak dose forecasts. The stepwise regression results are shown in Table 5. The four parameters selected, in order, are: k_{lith} , $one_over_alpha_A$, $Flow_Focusing_Factor$, and $k_{nonlith}$. The table shows the estimated regression coefficient and its standard error of estimation, the standardized regression coefficient, t-statistic, significance level, and 95% confidence interval for each regression coefficient. At the right of the table, the R-square for the regression, the adjusted R-square, and the change in R-square obtained by adding each additional parameter to the regression are shown. Note that the change (improvement) in R-square decreases rapidly after the first two parameters k_{lith} and $one_over_alpha_A$ are added to the regression.

The four parameters are measured in different units, therefore the values of the estimated regression coefficients vary markedly in magnitude. To avoid problems of units of measurement, the SPSS regression program provides estimates of the standardized regression coefficients. Before fitting the regression equation, all variables—the dependent and four explanatory variables—are standardized by subtracting the mean and dividing by the standard deviation. The standardized regression coefficients represent the change in the dependent variable for a change of one standard deviation in the explanatory variable. SPSS labels the standardized coefficients as "Beta" in Table 5, while the ordinary coefficients are labeled "B."

¹² Visit <http://www.spss.com/spss/> for more information on this statistical software.

The relative magnitude and direction of the standardized coefficients for the four seepage parameters are shown in Figure 12.

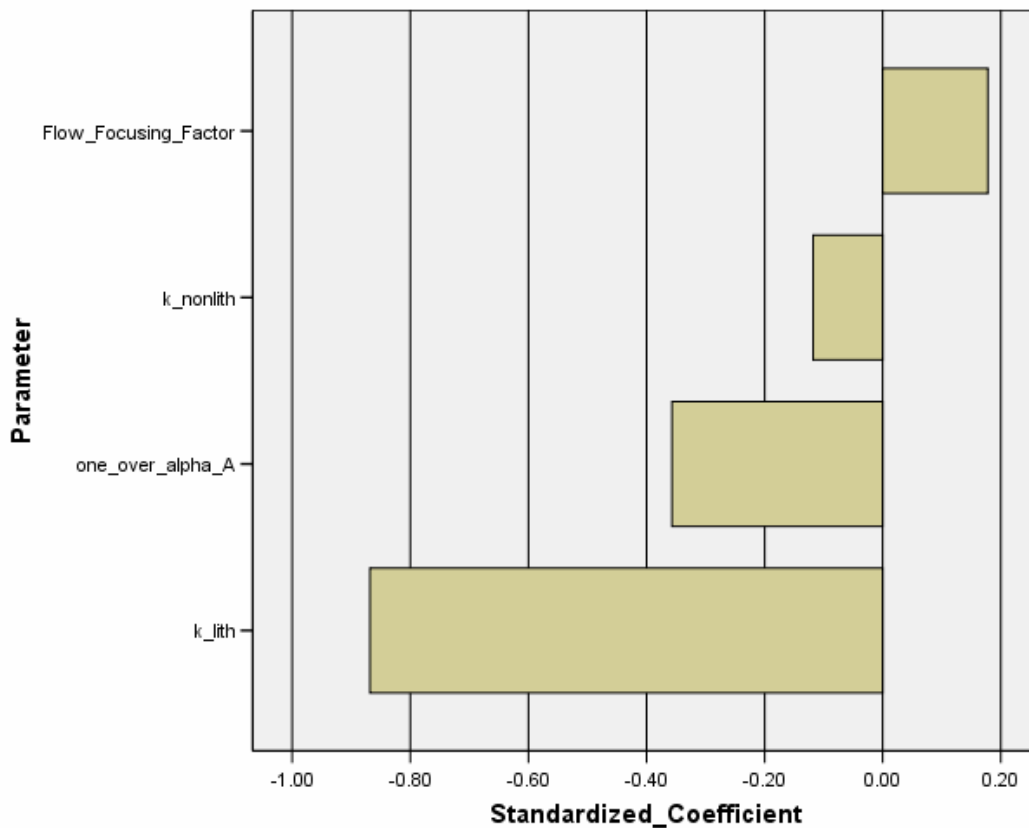


Figure 12. Standardized Coefficients for Seepage Parameters in Stepwise Regression of Annual Dose Maxima for Seepage Parameter Sensitivity Run with EPA Uncertainty Model
(N=1000 realizations, $R^2 = 0.885$) (Source: Run 5)

The standardized coefficients indicate that k_{lith} , the tangential fracture permeability in lithophysal units in the boundary layer near the drift wall, is the most important contributor to the variation in peak dose when only the variation in the four seepage parameters is included in the forecasted annual dose. This key parameter affects the diversion of water around the drifts. A higher value of tangential permeability diverts more water around the drift and reduces seepage onto the wastes. As expected, the sign of its standardized coefficient (beta) is negative, indicating that a change from its mean to a one standard deviation higher value of k_{lith} leads to a (logged) peak dose forecast that is approximately 0.9 standard deviations below its mean value. The variation in k_{lith} accounts for almost 71% of the variation in peak dose forecasts in Run 5.

Table 4. Characteristics of the Four Seepage Parameters Used in Stepwise Regression Procedure

Rank	Parameter_Name	Parameter_Description	GoldSim Module	Type Distribution	Mean	StdDev	Min	Max
1	<i>k_lith</i>	Tangential fracture permeability (lithophysal units)	\Drift_Seepage_Model	Triangular	-11.5	0.37559	-12.42	-10.58
2	<i>one_over_alpha_A</i>	Capillary strength above drift	\Drift_Seepage_Model	Triangular	591	42.866	486	696
3	<i>Flow_Focusing_Factor</i>	Seepage flow focusing factor	\Drift_Seepage_Model	Uniform	1.5	0.28868	1	2
4	<i>k_nonlith</i>	Tangential fracture permeability (non-lithophysal units)	\Drift_Seepage_Model	Triangular	-12.2	0.27761	-12.88	-11.52

Table 5. Coefficients and Statistics for Seepage Parameters Used in Stepwise Regression of Annual Dose Maxima for EPA Uncertainty Model

(N=1000 realizations, $R^2 = 0.885$) (Source: Run 5)

ID	Model Parameters in Order of Entry into SPSS Stepwise Regression Procedure	Unstandardized Coefficients ^a		Standardized Coefficients ^a	t-Statistic	Sig.	95% Confidence Interval for B		R Square	Adjusted R Square	R Square Change
		B	Std. Error	Beta			Lower Bound	Upper Bound			
0	(Constant)	-14.225	.356		-39.992	.000	-14.923	-13.527			
1	<i>k_lith</i>	-1.353	.017	-.868	-80.624	.000	-1.386	-1.320	.709	.708	.709
2	<i>One_over_alpha_A</i>	-.005	.000	-.356	-33.095	.000	-.005	-.005	.840	.840	.131
3	<i>Flow_Focusing_Factor</i>	.360	.022	.178	16.513	.000	.317	.403	.871	.871	.031
4	<i>k_nonlith</i>	-.249	.023	-.118	-10.994	.000	-.294	-.205	.885	.885	.014

a Dependent Variable: Log10_Maximum_Dose

The second parameter to enter the stepwise regression is *one_over_alpha_A*, the capillary strength ($1/\alpha$) in the zone near the drift crown. Larger values of capillary strength imply a greater capillary force, holding water in the fractures and reducing seepage. The standardized coefficients indicate that *one_over_alpha_A* is the second most important contributor to the variation in peak dose in Run 5. Its sign is also negative, indicating that higher values of *one_over_alpha_A* lead to lower peak doses. For example, a change from its mean to a one standard deviation higher value of *one_over_alpha_A* leads to a (logged) peak dose forecast that is approximately 0.35 standard deviations below its mean value. The variation in *one_over_alpha_A* accounts for an additional 13% of the variation in peak dose forecasts in Run 5 beyond that explained by *k_lith* alone.

The third parameter to enter the stepwise regression is *Flow_Focusing_Factor*, the seepage flow-focusing factor. The standardized coefficients indicate that the *Flow_Focusing_Factor* is the third most important contributor to the variation in peak dose in Run 5. Its sign is positive, indicating that higher values of *Flow_Focusing_Factor* lead to higher peak doses. The variation in *Flow_Focusing_Factor* only accounts for an additional 3% of the variation in peak dose forecasts in Run 5 beyond that explained by *k_lith* and *one_over_alpha_A*.

Although all four seepage parameters were found to be statistically significant contributors to the variation in peak dose forecasts in Run 5, the fourth parameter *k_nonlith*, the tangential fracture permeability in non-lithophysal units, explains an additional 1.4% of the variation in peak dose. It has the same sign and direction of effect as *k_lith*, but with smaller magnitude.

4.3 SENSITIVITY TO SOLUBILITY PARAMETERS

The EPA Uncertainty Model uses the same suite of radionuclides as used by DOE in the Peak Dose Model except for the previously noted additions of Tc-99 and I-129. The total suite of radionuclides assumed to be present in the initial inventory includes Am-241, Am-243, I-129, Np-237, Pa-231, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Tc-99, Th-229, Th-230, Th-232, U-233, U-234, U-235, U-236, and U-238. From an inventory perspective, Am-241 ($t_{1/2} = 4.33\text{E}+02$ yr) is assumed to have fully decayed to Np-237; Am-243 ($t_{1/2} = 7.37\text{E}+03$ yr) is assumed to have fully decayed to Pu-239; Pu-238 ($t_{1/2} = 8.77\text{E}+01$ yr) is assumed to have fully decayed to U-234; and Pu-241 ($t_{1/2} = 1.44\text{E}+01$ yr) is assumed to have fully decayed to Np-237 (OCRWM 2005, Table 35).

In addition to the enumerated radionuclides in the initial inventory, dose to the RMEI includes contributions from Ac-227, Ra-226, Ra-228, and Pb-210. These daughter products of Pa-231, Th-230, Th-232, and Ra-226, respectively, are assumed to be in secular equilibrium with their parent nuclides at the location of the RMEI. The daughter products have sufficiently short half-lives that any forming upstream of the receptor will have decayed away during transport.

Typically, the dissolved concentration limits are obtained from look-up tables that provide values, S , of the log of the dissolved concentration limits (mg/l) as a function of pH and the log of the fugacity of carbon dioxide ($f\text{CO}_2$) in bars. The look-up table value is adjusted for uncertainties in the thermodynamic properties data (ϵ_1) and uncertainties in fluoride concentrations in the percolating water (ϵ_2). For some elements, the uncertainty parameter, ϵ_2 , is

multiplied by a factor N, which is a function of pH. Both ϵ_2 and N may vary with the type of fuel (i.e., CSNF and CDSP). The dissolved concentration limit equations used in the EPA model are summarized in Table 6. The DOE source documents for the look-up tables and uncertainty parameters are also summarized in Table 6. It should be noted the thermodynamic data used for calculating the solubilities are based on a temperature of 25° C and that the actinide solubilities decrease with decreasing temperature (BSC 2004a, Section 6.3.3.3). Since this temperature will not be reached until about 100,000 years, the solubilities are conservatively calculated.

Table 6. Modeling Parameters for Radionuclide Solubility

Element	Dissolved Concentration Limits Equation	Reference
Np	$\log[\text{Np}] = S(\text{pH}, \log f\text{CO}_2) + \epsilon_1 + (\epsilon_2 \times \text{N})$	Tables 37, 38, and 39 – OCRWM 2005
Pu	$\log[\text{Pu}] = S(\text{pH}, \log f\text{CO}_2) + \epsilon_1 + (\epsilon_2 \times \text{N})$	Tables 42, 43, and 44 – OCRWM 2005
U	$\log[\text{U}] = S(\text{pH}, \log f\text{CO}_2) + \epsilon_1 + (\epsilon_2 \times \text{N})$	Tables 48, 49, 50, and 51 – OCRWM 2005
Pa	$\log[\text{Pa}] = S(\text{pH}, \log f\text{CO}_2) + \epsilon_1 + \epsilon_2$	Tables 40 and 41 – OCRWM 2005
Th	$\log[\text{Th}] = S(\text{pH}, \log f\text{CO}_2) + \epsilon_1 + \epsilon_2$	Tables 46 and 47 – OCRWM 2005
Tc	Not solubility limited	Section 6.14 – BSC 2004a
I	Not solubility limited	Section 6.14 – BSC 2004a

No solubility-limiting phases are expected for Tc and I (BSC 2004a.) Consequently, solubility is not defined for these elements; rather the release of Tc and I to the percolating ground water is assumed to be controlled by the rate of dissolution of the waste forms within the waste packages. As noted previously, DOE conservatively assumes in the Peak Dose Model that, once the waste package is breached, the waste forms are fully degraded and all radionuclides are available for transport (OCRWM 2005, Section 4.2.7). Thus, release of Tc and I would be immediate and total for breached waste packages. This assumption, consistent with the DOE modeling, is reasonable since I and Tc removal, if not solubility limited, would be controlled by the dissolution rate of the waste matrix. In reality, radionuclides in breached waste packages would be released gradually, and the mean dose at 10,000 years would be lower than predicted here for the assumed failure of 520 waste packages. Alternatively, more early failures must be assumed to achieve a mean dose of 15 mrem/yr at 10,000 years.

Values of $f\text{CO}_2$ and pH used to define solubility values in the look-up tables depend on water chemistry. As noted above, in the Peak Dose Model, DOE assumed five equally probable water chemistries (OCRWM 2005, Section 4.2.3.2). Look-up tables for each water chemistry presenting CO_2 partial pressure in the drifts and inverts as a function of time are included in *Engineered Barrier System: Physical and Chemical Environment*, Tables 6.7-1 through 6.7.5 (BSC 2004c). The final time step in each look-up table covers the period 17,511.5 to 100,000 years. Carbon dioxide partial pressure data for this final time step are used in the DOE Peak Dose Model (OCRWM 2005, Table 6). Use of the same data in the EPA Uncertainty Model is a reasonable choice, as will be discussed below.

For the first 600 years after waste package failure, the in-package pH for CSNF waste packages varies from a minimum value of 4.5 to a maximum value ranging from 7.0 to 8.1. The maximum

value is a function of $f\text{CO}_2$. For the period from 600 to 20,000 years after waste package failure, the pH in CSNF waste packages is assigned a uniform distribution ranging from 4.5 to 7.0 independent of $f\text{CO}_2$ (OCRWM 2005, Table 8). For CDSP waste packages, the in-package pH is assigned a uniform distribution of 4.5 to 7.0 for flow rates of water into the waste packages of ≤ 150 l/yr, while the distribution is broadened to pH 4.5 to 8.0 for water in-flows of >150 l/yr. These distributions cover the period from 0 to 20,000 years after CDSP waste package breach (OCRWM 2005, Table 8).

The sensitivity of the EPA Baseline doses to uncertainty in the solubility parameters in Table 6 was examined in a test where all parameters except radionuclide solubility parameters were set at mean values, and the *Starting_Water_Chemistry* discrete parameter¹³ was set at the CS1000 chemistry (OCRWM 2005, Table 6), as it had been in all the sensitivity cases discussed above. The solubility parameters were allowed to vary over the full range of their assigned distributions. Results presented in Figure 13 show that the mean peak dose based on 1,000 realizations reaches 442 mrem/yr at 92,000 years. The spread between the 5th and 95th percentiles ranges from 3.7 mrem/yr to 12 mrem/yr at 10,000 years, and increases to a range of 13 mrem/yr to 2,289 mrem/yr at the time of the peak for the 95th percentile (84,000 years), indicative of a substantial increase in uncertainty over time. Comparison of Figures 10 and 13 indicates that the uncertainty in solubility parameters is a significantly greater contributor to total dose uncertainty than the uncertainty in seepage factors. Essentially all of the uncertainty at the time of the peak dose is due to uncertainty in plutonium solubility.

In this sensitivity run, fixed parameters in the EPA Uncertainty Model include time of waste package failure set at 2,500 years, *Starting_Water_Chemistry* discrete parameter set at the CS1000 chemistry, pH for CSNF waste packages set at 5.75, and $f\text{CO}_2$ for the drifts set at $5.59 \text{ E-}3$ bars. As noted above, this value of $f\text{CO}_2$ is for the period 17,511.5 to 100,000 years. To evaluate whether the use of the 17,511.5 to 100,000 time period instead of a time period that embraces the waste package failure time of 2,500 years significantly affects the results, a value of CO_2 partial pressure was obtained for CS1000 water from Table 6.7-3 of BCS 2004c for the period 2,397 to 2,702 years. Since radionuclides of Pu are major contributors to dose (see Section 3.2), the solubility of Pu was determined from Table 42 of OCRWM 2005 for a pH of 5.75 using values of $f\text{CO}_2$ for 2,397 to 2,702 years and 17,511.5 to 100,000 years. For the early time period, the solubility was 0.093 mg/l, while for the later period, the solubility was 0.11 mg/l. This indicates that the use of data for the longer time period will have limited impact on the results obtained with the EPA Uncertainty Model.

Two additional sensitivity tests were made. In the first, the *Starting_Water_Chemistry* discrete parameter was allowed to vary over the five different chemistries included in the DOE Peak Dose Model, instead of being held fixed at the CS1000 chemistry. In the second, the *Cracks_Before_Patches* was also allowed to vary by assuming that this condition occurred in 50% of the realizations instead of in all the realizations, as is the case for the EPA Baseline. Neither of these additional tests yielded significant differences from the case where only the solubility was varied with a fixed starting water chemistry. Results of the three runs are compared in Table 7.

¹³ Five equi-probable starting water chemistries were used in the DOE Peak Dose Model.

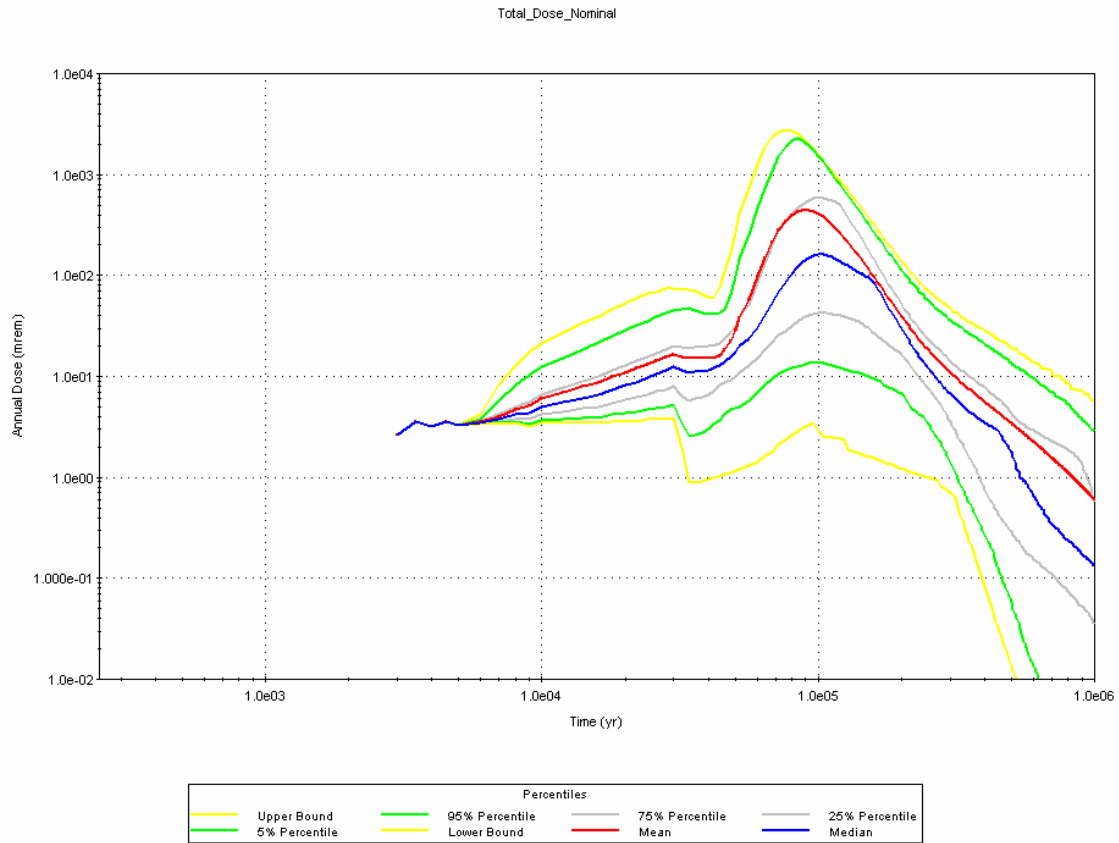


Figure 13. Mean and Selected Percentiles Showing Sensitivity of Total Annual Dose to Radionuclide Solubility Uncertainty/Variability

(Sensitivity analysis using EPA Uncertainty Model with all parameters at mean except for all solubility parameters, which range over their entire distributions. 520 WPs with early failure at 2,500 yr, 1,000 realizations, Infiltration case=2 (Medium).) (Source: Run 6)

Table 7. Sensitivity of EPA Baseline to Solubility Cases
(Source: Run 6)

Case	Mean Dose at 10,000 yr (mrem/yr)	Peak Mean Dose (mrem/yr)	Time of Mean Peak Dose (yr)
EPA Baseline with fixed <i>Starting_Water_Chemistry</i> and full stochastic variation in radionuclide solubility	6.0	442	92,000
EPA Baseline with variable <i>Starting_Water_Chemistry</i> and full stochastic variation in radionuclide solubility	5.9	433	88,000
EPA Baseline with variable <i>Starting_Water_Chemistry</i> , variable <i>Cracks_Before_Patches</i> and full stochastic variation in radionuclide solubility	5.9	414	92,000

4.3.1 Regression Analyses for Solubility Related Parameters

A stepwise regression procedure was also used to determine the relative importance of 16 solubility parameters in terms of their contribution to variations in forecasted annual dose shown in Figure 13. The data for the stepwise analysis are the 1,000 realizations from Run 6. The peak dose forecasts from this sensitivity run were obtained by fixing all model parameters other than the 16 solubility parameters at their mean value. The dependent variable for the stepwise regression procedure is the base-10 logarithm of the peak dose achieved over the 1,000,000-year time period.

The solubility parameters are the 16 explanatory variables in the regression, which also includes a constant term. The four solubility parameters evaluated by the stepwise regression procedure as most important are shown in Table 8. The table shows the name, description, location in the GoldSim model, and the distribution assigned for each solubility parameter. The stepwise regression results are shown in Table 9. The four parameters selected, in order, are *Log_Pu_Sol_eps1*, *Log_Np_Sol_eps1_NpO2*, *Log_U_Sol_eps1*, and *Log_Pa_Sol_eps2_CDSP*. The table shows the estimated regression coefficient and its standard error of estimation, the standardized regression coefficient, t-statistic, significance level, and 95% confidence interval for each regression coefficient. At the right of the table, the R-square for the regression, the adjusted R-square, and the change in R-square obtained by adding each additional parameter to the regression are shown. Note that the improvement in R-square decreases very rapidly after the first parameter, *Log_Pu_Sol_eps1* (the uncertainty in Pu solubility thermodynamics), is added to the regression, achieving an R-square of 0.973.

Table 8. Characteristics of the Four Solubility Parameters Selected by Stepwise Regression Procedure

Rank	Parameter_Name	Parameter_Description	GoldSim Module	Type Distribution	Mean	StdDev	Min	Max
1	<i>Log_Pu_Sol_eps1</i>	Uncertainty in solubility thermodynamics (Pu)	\Source_Term_Models	TruncNormal	0	1	-2	2
2	<i>Log_Np_Sol_eps1_NpO2</i>	Uncertainty in solubility thermodynamics (NpO ₂)	\Source_Term_Models	TruncNormal	0	0.6	-1.2	1.2
3	<i>Log_U_Sol_eps1</i>	Uncertainty in solubility thermodynamics (U)	\Source_Term_Models	Normal	0	0.5	-1.E+32	1.E+32
4	<i>Log_Pa_Sol_eps2_CDSP</i>	Uncertainty in solubility due to flourides (Pa)	\Source_Term_Models	Triangular	1.93	1.3647	0	5.79

Table 9. Coefficients and Statistics for Parameters Accepted in Stepwise Regression of Annual Dose Maxima versus 16 Stochastic Solubility Parameters Used in EPA Uncertainty Model
(N=1000 realizations, R² = 0.975) (Source: Run 6)

ID	Model Parameters in Order of Entry into SPSS Stepwise Regression Procedure	Unstandardized Coefficients ^a		Standardized Coefficients ^a	t-Statistic	Sig.	95% Confidence Interval for B		R Square	Adjusted R Square	R Square Change
		B	Std. Error	Beta			Lower Bound	Upper Bound			
0	(Constant)	2.221	.006		378.087	.000	2.209	2.232			
1	<i>Log_Pu_Sol_eps1</i>	.759	.004	.985	196.884	.000	.751	.766	.973	.973	.973
2	<i>Log_Np_Sol_eps1_NpO2</i>	.050	.006	.039	7.825	.000	.038	.063	.975	.975	.001
3	<i>Log_U_Sol_eps1</i>	.028	.007	.020	4.058	.000	.014	.041	.975	.975	.000
4	<i>Log_Pa_Sol_eps2_CDSP</i>	.006	.002	.012	2.433	.015	.001	.011	.975	.975	.000

a Dependent Variable: Log10_Maximum_Dose

The standardized coefficients indicate that *Log_Pu_Sol_eps1*, the uncertainty in Pu solubility thermodynamics, is the most important contributor to the variation in peak dose when only the variation in the 16 solubility parameters is included in the forecasted annual dose. Its sign is positive, indicating that a change from its mean to a one standard deviation higher value of *Log_Pu_Sol_eps1* leads to a (logged) peak dose forecast that is approximately 0.99 standard deviations above its mean value. The variation in *Log_Pu_Sol_eps1* accounts for over 97% of the variation in peak dose forecasts in Run 6.

The remaining three parameters to enter the stepwise regression are *Log_Np_Sol_eps1_NpO2*, *Log_U_Sol_eps1*, and *Log_Pa_Sol_eps2_CDSP*, which are the uncertainty in NpO₂ solubility thermodynamics, the uncertainty in U solubility thermodynamics, and the uncertainty in Pa solubility due to fluorides, respectively. These three parameters have small, positive standardized coefficients. The relative magnitude and direction of the estimated standardized coefficients for the four selected solubility parameters are shown in Figure 14.

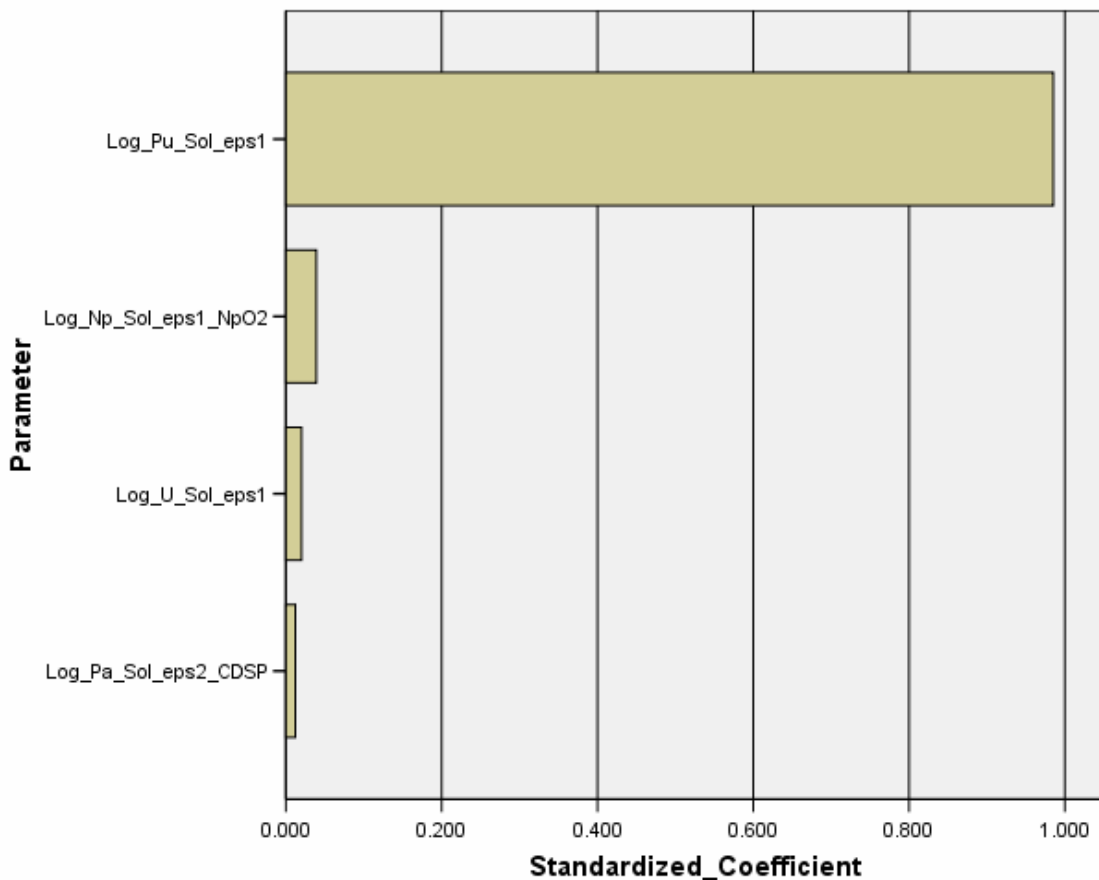


Figure 14. Standardized Coefficients of Four Most Significant Solubility Parameters in Stepwise Regression of Annual Dose Maxima for Solubility Parameter Sensitivity Run with EPA Uncertainty Model
(N=1000 realizations, $R^2 = 0.975$) (Source: Run 6)

4.4 COMBINED SENSITIVITIES

The effect of varying both the seepage and solubility parameters over their full stochastic ranges while holding other parameters at the mean was also evaluated. Figure 15 shows the impact on dose to the RMEI of varying both seepage parameters and solubility parameters over the full range while holding all other parameters at their mean values. The combined results show a peak mean dose of 499 mrem/yr, while the peak mean dose was 442 mrem/yr when only the solubility parameters were varied (Figure 13), and 183 mrem/yr when only the seepage factors were varied (Figure 11). These values are all higher than the Baseline dose of 163 mrem/yr forecasted by the EPA Uncertainty Model with all parameters fixed at their means. Introducing stochastic variation in the parameters, rather than using their mean values, increases the mean annual dose in all three cases.

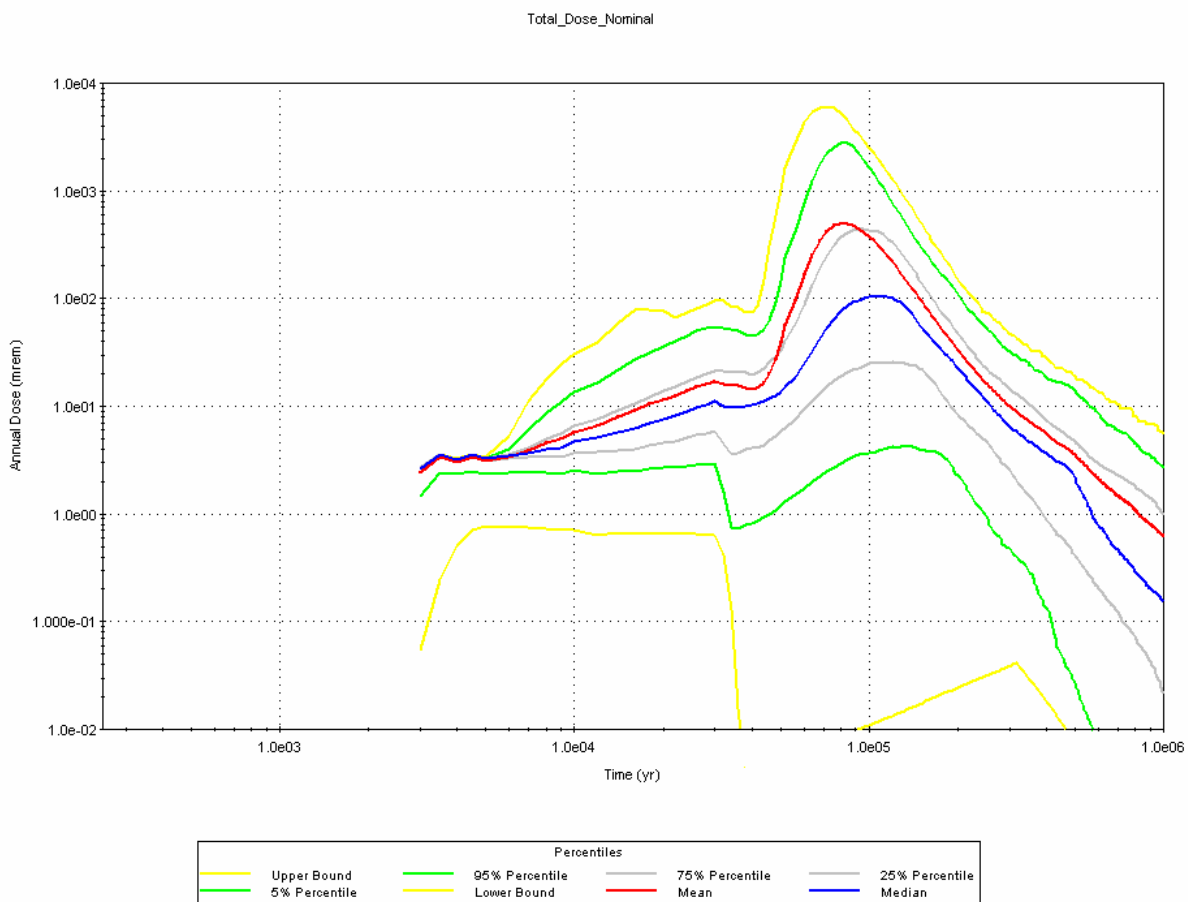


Figure 15. Annual Dose versus Time for Cases Where Seepage and Solubility Parameters are Varied Simultaneously Over Assigned Ranges, with All Other Parameters Held at Mean Values
(Source: Run 7)

Since seepage and solubility effects are coupled to the infiltration rate, a sensitivity test was made in which seepage factors, infiltration rates, and solubilities were all allowed to vary stochastically while holding other parameters at their mean values. Results are shown in Figures 16, 17, 18, and 19. Figure 16 illustrates the spread between the 5th and 95th percentiles when seepage parameters and solubility parameters are each allowed to vary individually, and when seepage parameters, solubility parameters, and infiltration rates are allowed to vary in combination with all other parameters held at their mean values. The trend of increasing uncertainty between the time of initial waste package failures to the time of the peak dose is indicated by the increasing spread between the 5th and 95th percentile curves in Figure 16.

The mean annual dose when seepage parameters and solubility parameters are each allowed to vary individually; when seepage parameters, solubility parameters, and infiltration rates are allowed to vary in combination; and when all parameters are allowed to vary are compared with the EPA Baseline in Figure 17. Figure 18 shows the difference of each mean dose from the EPA Baseline. Varying seepage parameters show only a small change in mean dose from the EPA Baseline, with a slightly higher and earlier peak dose. Varying solubility generates a much larger increase in the peak mean dose, and introducing variation in infiltration produces an additional increase in the peak dose. When all parameters are allowed to vary, the peak dose is reduced and moved closer in time. The other parameters introducing variability at this stage include a large number of K_d coefficients, which spread the release and migration of radionuclides over time and reduce the peak mean dose.

The median annual dose when seepage parameters and solubility parameters are each allowed to vary individually; when seepage parameters, solubility parameters, and infiltration rates are allowed to vary in combination; and when all parameters are allowed to vary are compared with the EPA Baseline in Figure 19. Although the introduction of variability generated increases in the mean dose, the addition of variability serves to reduce the median dose when compared with the EPA Baseline. When seepage or solubility parameters are varied, the reduction in median dose is small. But when infiltration is permitted to vary, the median dose is reduced more appreciably. This reduction in median dose is due to the 24% probability assigned to the Low Infiltration case. When only seepage and solubility parameters are varied, the infiltration rate is fixed to the medium infiltration case. When only solubility or seepage parameters are varied, the peak median dose is 160 or 161 mrem/yr, respectively; slightly below the EPA Baseline peak of 163 mrem/yr. When seepage, solubility, and infiltration rates are varied simultaneously, the peak median dose is reduced approximately in half to 87 mrem/yr. Allowing variation in all parameters results in a much lower median annual dose, with a peak of 27 mrem/yr.

Statistics comparing the uncertainties in various sensitivity runs are shown in Table 10 and are compared to the case where all parameters are allowed to vary over the full range specified in the DOE Peak Dose Model.¹⁴ Since the peak in the 5th and 95th percentile curves of annual doses-versus-time do not occur at the same time, comparisons are made using the values of the 5th percentile at the time the 95th percentile reaches its peak.

¹⁴ For the seepage, solubility, and infiltration cases, the waste package failure time was fixed at 2,500 years, while for the case where all parameters were varied, the failure times were uniformly distributed from 0 to 5,000 years.

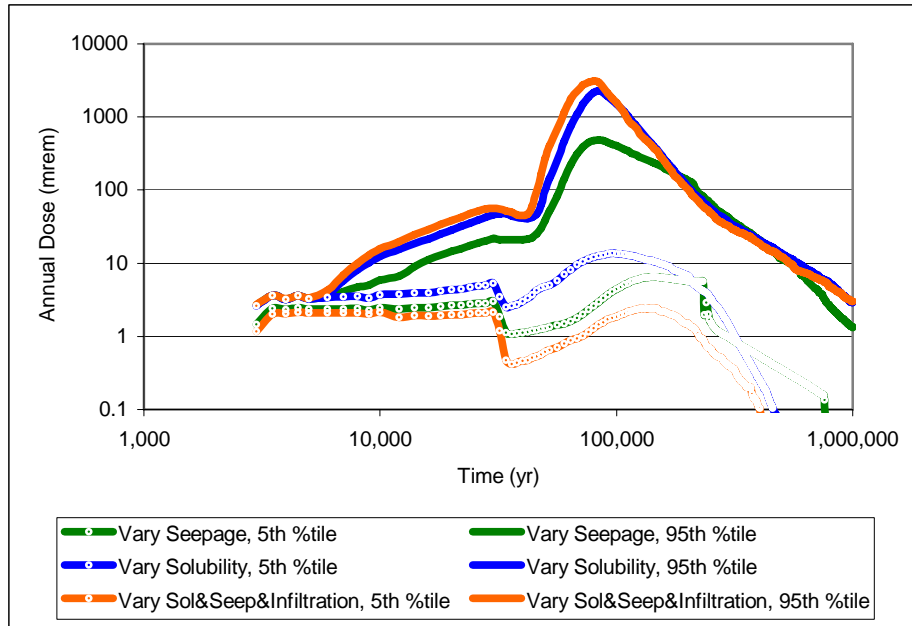


Figure 16. Comparison of Sensitivity Tests Showing Uncertainty Ranges When Seepage Parameters and Solubility Parameters are Each Allowed to Vary Independently, and When Seepage, Solubility, and Infiltration Rates are Varied in Combination
 (Source: Runs 5, 6, and 8)

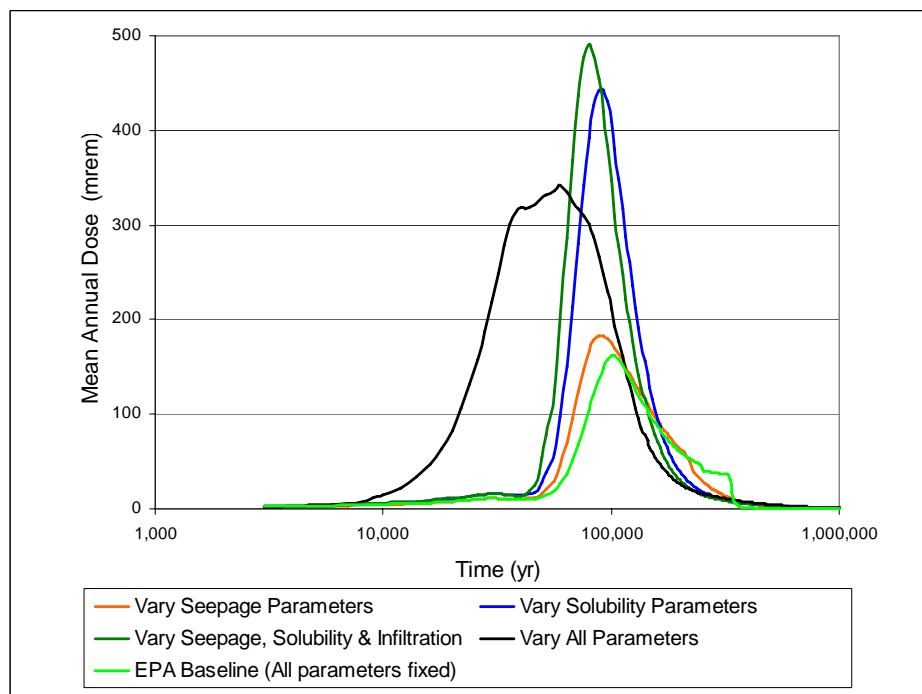


Figure 17. EPA Baseline Compared with Mean Value of Sensitivity Tests When Seepage Parameters and Solubility Parameters are Each Allowed to Vary Independently; When Seepage, Solubility, and Infiltration Rates are Varied in Combination; and When All Parameters Vary
 (Source: Runs 1, 2, 5, 6, and 8)

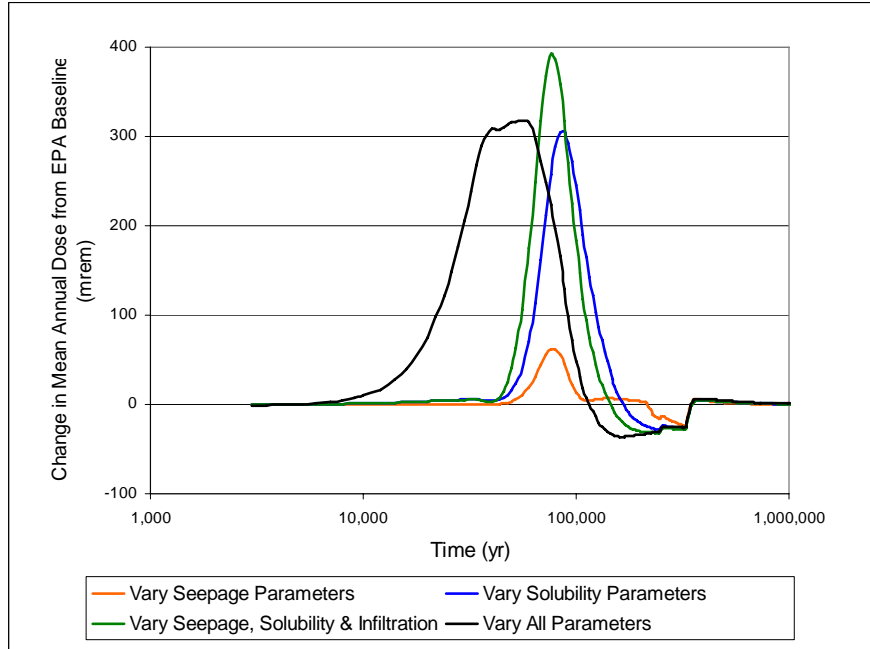


Figure 18. Difference in Mean Dose from EPA Baseline When Seepage Parameters and Solubility Parameters are Each Allowed to Vary Independently; When Seepage, Solubility, and Infiltration Rates are Varied in Combination; and When All Parameters are Varied
 (Source: Runs 1, 5, 6, and 8)

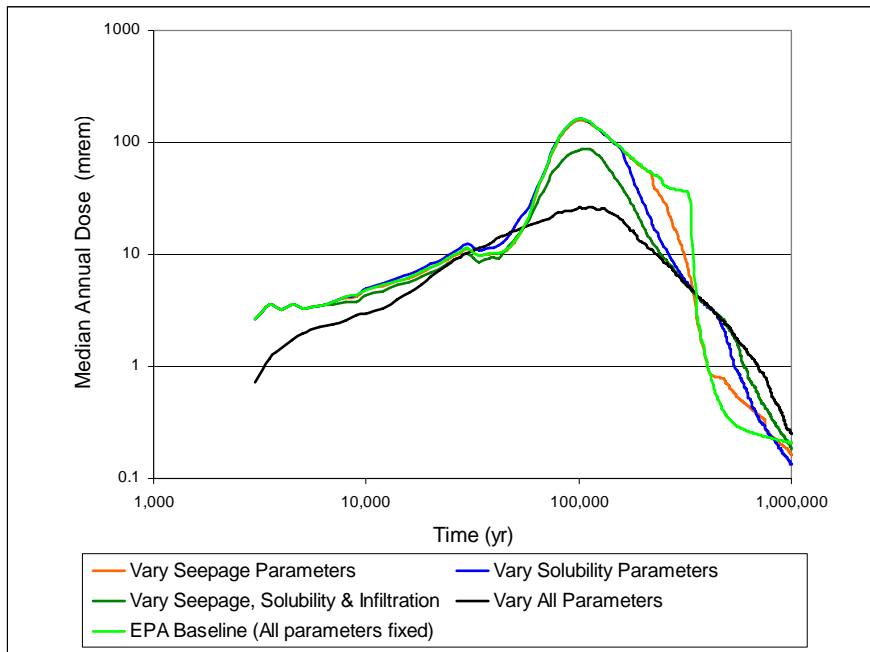


Figure 19. EPA Baseline Compared with Median Value of Sensitivity Tests When Seepage Parameters and Solubility Parameters are Each Allowed to Vary Independently; When Seepage, Solubility, and Infiltration Rates are Varied in Combination; and When All Parameters Vary
 (Source: Runs 1, 2, 5, 6, and 8)

Table 10. Statistics Measuring Uncertainty in Various Sensitivity Cases
(Doses in mrem/yr) (Source: Runs 1, 5, 6, and 8)

Statistic		Vary Solubility	Vary Seepage	Vary Seepage, Solubility, and Infiltration Rate	Vary All Parameters
5 th percentile	Peak Dose	13.7	6.5	2.4	1.0
	Year of Peak Dose	96,000	144,000	144,000	22,000
Mean	Peak Dose	442	183	491	342
	Year of Peak Dose	92,000	92,000	80,000	60,000
Median	Peak Dose	161	160	87.1	26.6
	Year of Peak Dose	100,000	104,000	112,000	112,000
95 th percentile	Peak Dose	2,288	485	3,089	1,972
	Year of Peak Dose	84,000	84,000	80,000	64,000
5 th percentile. (At year of peak of 95 th percentile)		12.6	3.0	1.3	0.6
Range Ratio (95 th /5 th)		181	162	2,387	3,049
Orders of Magnitude Spread in Range Ratio ^a		2.3	2.2	3.4	3.5

a - log base 10 of range ratio

From Table 10, it can be discerned that the uncertainty associated with seepage parameter and solubility parameter variability is about the same (i.e., the Range Ratios and order of magnitude spreads are about the same). However, variability in solubility parameters leads to higher annual doses than the variability in seepage parameters. Adding variability in the infiltration rate causes a large increase in the Range Ratio (about 15-fold).

The case where seepage parameters, solubility parameters, and infiltration rates are allowed to vary (Column 4) versus the case where all parameters are allowed to vary (Column 5) shows a slightly lower Range Ratio for the former. However, the 5th percentile, mean, and 95th percentile are lower for the case where all parameters are allowed to vary. The fact that the two cases have similar range ratios indicates that most of the uncertainty is captured by these three groups of parameters. It must be remembered that, with the EPA Uncertainty Model, uncertainties associated with waste package and drip shield behavior are eliminated.

By comparing the range ratio (95th/5th) data at the time of the peak dose from Table 10 with the equivalent range ratios at 10,000 years, one can obtain an estimate of the extent that uncertainty increases with time. The following tabulation provides such a comparison:

<u>Sensitivity Case</u>	<u>Range Ratio at Peak/Range Ratio at 10,000 yr</u>
Vary Solubility	181/3.35 = 54.0
Vary Seepage	162/2.32 = 23.3
Vary Seep. Sol. & Infil.	2,387/7.52 = 317
Vary All Parameters	3,049/34.0 = 89.7

The increase in the range ratio over the period from 10,000 years to the time of the peak dose clearly demonstrates the large temporal increase in uncertainty. For the case where all parameters are varied, the increase is about two orders of magnitude from 10,000 years to the time of the peak dose

The SPSS stepwise regression procedure was used to determine the relative importance of the seepage, solubility, and infiltration parameters in terms of their contribution to the variation in forecasted annual dose shown in Figure 16. The data for the stepwise analysis are the 1,000 realizations from Run 8. The peak dose forecasts from this sensitivity run were obtained by fixing all parameters other than the 21 solubility, seepage, and infiltration parameters at their mean values.

The stochastic infiltration rate element in GoldSim is a discrete choice variable, taking values 1, 2, or 3 for low, medium, and high infiltration rate scenarios, respectively. This variable was replaced by repository long-term average infiltration rate variable (the real-valued GoldSim function element *Repos_Avg_Infil_LTA*) for the regression analysis. The three values of this regression variable are the three plateau levels shown at the right in Figure 2. Each realization has one of the three plateau levels assigned, with probabilities 0.24, 0.41, and 0.35 for the low, medium and high infiltration rate scenarios, respectively.

The dependent variable for the stepwise regression procedure is the base-10 logarithm of the peak dose achieved over the 1,000,000-year time period. The set of seepage, solubility, and infiltration parameters are the 21 explanatory variables in the regression, which also includes a constant term.

The eight parameters selected by the stepwise regression procedure are shown in Table 11. The table shows the name, description, location in the GoldSim model, and the distribution assigned for each parameter. The stepwise regression results are shown in Table 12. The table shows the estimated regression coefficient and its standard error of estimation, the standardized regression coefficient, t-statistic, significance level, and 95% confidence interval for each regression coefficient. At the right of the table, the R-square for the regression, the adjusted R-square, and the change in R-square obtained by adding each additional parameter to the regression are shown.

Table 11. Characteristics of the Eight Seepage, Solubility, and Infiltration Parameters Selected by Stepwise Regression Procedure

Rank	Parameter_Name	Parameter_Description	GoldSim Module	Type Distribution	Mean	StdDev	Min	Max
1	<i>Log_Pu_Sol_eps1</i>	Uncertainty in solubility thermodynamics (Pu)	\Source_Term_Models	TruncNormal	0	1	-2	2
2	<i>k_lith</i>	Fracture permeability (lithophysal units)	\Drift_Seepage_Model	Triangular	-11.5	0.37559	-12.42	-10.58
3	<i>Repos_Avg_Infil_LTA</i>	Repository longterm average infiltration rate	\Infiltration_Model	Discrete	2	1	1	3
4	<i>one_over_alpha_A</i>	Capillary strength above drift	\Drift_Seepage_Model	Triangular	591	42.866	486	696
5	<i>Flow_Focusing_Factor</i>	Seepage flow focusing factor	\Drift_Seepage_Model	Uniform	1.5	0.28868	1	2
6	<i>k_nonlith</i>	Fracture permeability (non-lithophysal units)	\Drift_Seepage_Model	Triangular	-12.2	0.27761	-12.88	-11.52
7	<i>Log_Np_Sol_eps1_NpO2</i>	Uncertainty in solubility thermodynamics (NpO ₂)	\Source_Term_Models	TruncNormal	0	0.6	-1.2	1.2
8	<i>Log_Np_Sol_eps2_NpO2_CDSP_I</i>	Uncertainty in solubility due to flourides (NpO ₂)	\Source_Term_Models	Triangular	0.29567	0.20907	0	0.887

Table 12. Coefficients and Statistics for Parameters Accepted in Stepwise Regression of Annual Dose Maxima versus 21 Stochastic Seepage, Solubility, and Infiltration Parameters Used in EPA Uncertainty Model
(N=1000 realizations, R² = 0.893) (Source: Run 8)

ID	Model Parameters in Order of Entry into SPSS Stepwise Regression Procedure	Unstandardized Coefficients ^a		Standardized Coefficients ^a	t-Statistic	Sig.	95% Confidence Interval for B		R Square	Adjusted R Square	R Square Change
		B	Std. Error	Beta			Lower Bound	Upper Bound			
0	(Constant)	-12.941	.533		-24.290	.000	-13.986	-11.895			
1	<i>Log_Pu_Sol_eps1</i>	.677	.011	.656	62.887	.000	.656	.698	.436	.435	.436
2	<i>K_lith</i>	-1.194	.025	-.494	-47.521	.000	-1.243	-1.145	.670	.670	.235
3	<i>Repos_Avg_Infil_LTA</i>	.024	.001	.407	39.140	.000	.023	.025	.832	.831	.161
4	<i>one_over_alpha_A</i>	-.004	.000	-.209	-20.128	.000	-.005	-.004	.877	.876	.045
5	<i>Flow_Focusing_Factor</i>	.309	.033	.098	9.467	.000	.245	.374	.887	.886	.010
6	<i>K_nonlith</i>	-.219	.034	-.067	-6.453	.000	-.286	-.152	.891	.891	.005
7	<i>Log_Np_Sol_eps1_NpO2</i>	.070	.018	.040	3.884	.000	.034	.105	.893	.892	.002
8	<i>Log_Np_Sol_eps2_NpO2_CDSP_I</i>	-.114	.045	-.026	-2.526	.012	-.203	-.026	.893	.893	.001

a Dependent Variable: Log10_Maximum_Dose

The eight selected parameters are *Log_Pu_Sol_eps1*, *k_lith*, *Repos_Avg_Infil_LTA*, *one_over_alpha_A*, *Flow_Focusing_Factor*, *k_nonlith*, *Log_Np_Sol_eps1_NpO2*, and *Log_Np_Sol_eps2_NpO2_CDSP_I*. Note that the improvement in R-square decreases after the three parameters *Log_Pu_Sol_eps1*, *k_lith*, and *Repos_Avg_Infil_LTA* are added to the regression, achieving an R-square of 0.832. The first two of the top three, the uncertainty in Pu solubility thermodynamics and the fracture permeability in lithophysal units, were previously selected as the most important parameters in separate analyses of seepage and solubility parameter sensitivity in Sections 4.2 and 4.3. Furthermore, these two parameters are also selected as the two most important in the analysis of the variation due to all model parameters, presented in the following section. Addition of the next two variables, *one_over_alpha_A* and *Flow_Focusing_Factor*, increases the R-square to 0.887. The first four parameters selected in this stepwise regression are all included among the first five parameters selected from all model parameters in the following section. The final three parameters add little additional explanatory power. The relative magnitude and direction of the estimated standardized coefficients for the eight selected parameters are shown in Figure 20.

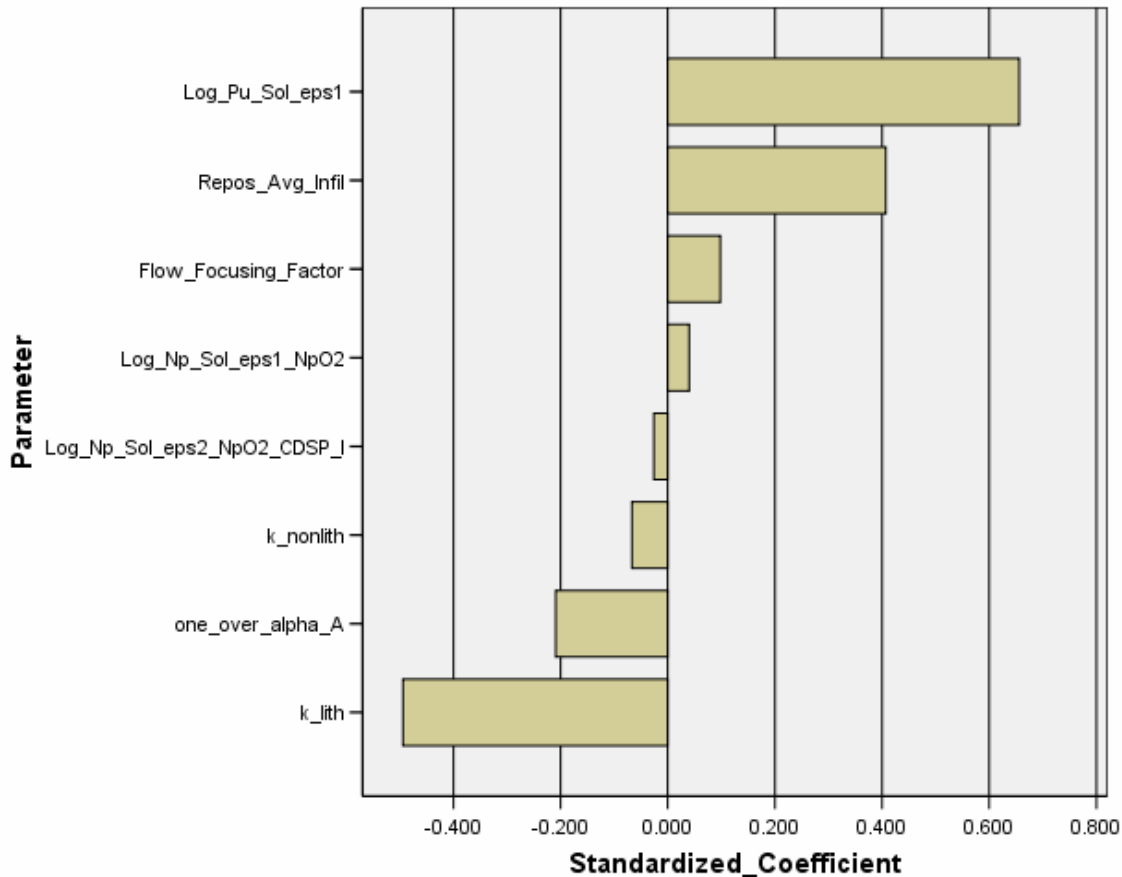


Figure 20. Standardized Coefficients of Eight Most Significant Parameters in Stepwise Regression of Annual Dose Maxima versus 21 Stochastic Seepage, Solubility, and Infiltration Parameters used in EPA Uncertainty Model
(N=1000 realizations, $R^2 = 0.893$) (Source: Run 8)

4.5 STEPWISE REGRESSION ANALYSIS OF ALL MODEL PARAMETERS

The stepwise regression procedure was applied to determine the relative importance of all 76 parameters in the model in terms of their contribution to the variation in the baseline forecasted annual dose shown in Figure 9. The data for the stepwise analysis are the 1,000 realizations from Run 1. The peak dose forecasts were from the EPA Uncertainty Model, with all stochastic parameters in the model varying over their assigned distribution. The 1,000 realizations are shown in Figure 21. Plots of the mean and selected statistics derived from the 1,000 realizations were shown previously in Figure 4. The mean annual dose at 10,000 years, averaged over all 1,000 realizations, is approximately 15 mrem/yr. As noted in Table 10, the mean annual dose reaches a peak of 342 mrem/yr at 60,000 years. At that time, the variation across the 1,000 realizations shown in Figure 21 is over five orders of magnitude from lowest to highest, with 839 (83.9%) realizations less than the mean of 342 mrem/yr.

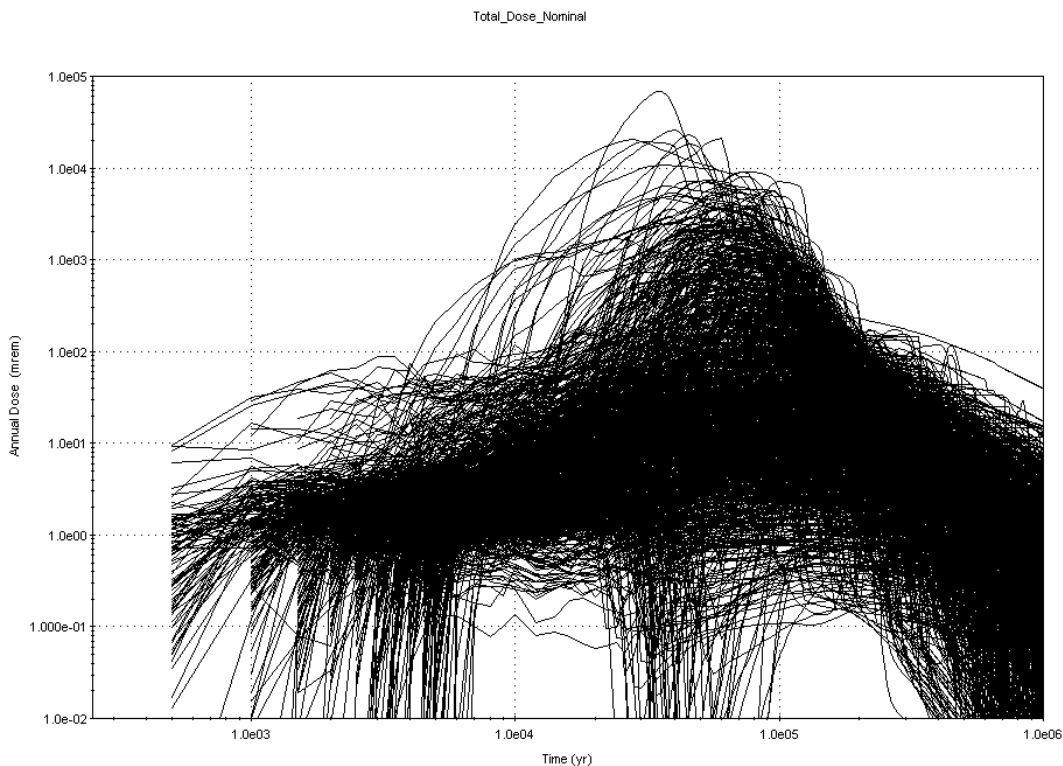


Figure 21. Total Annual Dose, 1,000 Realizations with EPA Uncertainty Model
(Source: Run 1)

The distribution of annual dose forecasts at 60,000 years is highly skewed to the right. The mean is near the 84th percentile of the distribution because of the large influence that the 10 (1%) highest realizations have on the arithmetic mean. These highly influential realizations are seen at the top of the plot in Figure 21. In contrast, there are 228 (22.8%) realizations with a peak dose less than 15 mrem/yr over the entire 1,000,000-year analysis period.

The dependent variable for the stepwise regression procedure is the base-10 logarithm of the peak dose achieved for each realization over the 1,000,000-year time period.

All 76 parameters are used as the explanatory variables in the regression, which also includes a constant term. The 76 parameters include the 21 used in Section 4.4 and 55 other parameters listed in Appendix B (Table B-3). The 22 parameters selected by the stepwise regression procedure are shown in Table 13. The table shows the name, description, location in the GoldSim model, and the distribution assigned for each selected parameter. The stepwise regression results are shown in Table 14. The table shows the estimated regression coefficient and its standard error of estimation, the standardized regression coefficient, t-statistic, significance level, and 95% confidence interval for each regression coefficient. At the right of the table, the R-square for the regression, the adjusted R-square, and the change in R-square obtained by adding each additional parameter to the regression are shown. Note that the first five parameters selected in Table 14 include the first four parameters listed in Table 12; *Log_Pu_Sol_eps1*, *k_lith*, *Repos_Avg_Infil_LTA*, and *one_over_alpha_A*. The first five parameters achieve an R-square of over 70%, with a sharp reduction in the improvement obtained after the top five. Of the top five parameters, the only parameter not previously discussed is *GWSPD*, the ground-water specific discharge multiplier in the SZ.¹⁵ This parameter is also infiltration related.

The standardized coefficients indicate that *Log_Pu_Sol_eps1*, the uncertainty in Pu solubility thermodynamics, is again the most important contributor to the variation in peak dose when variation in all model parameters is included in the forecasted annual dose. Its sign is positive, indicating that a change from its mean to a one standard deviation higher value of *Log_Pu_Sol_eps1* leads to a (logged) peak dose forecast that is approximately 0.53 standard deviations above its mean value. The variation in *Log_Pu_Sol_eps1* accounts for over 28% of the variation in peak dose forecasts in Run 1.

The next parameter to enter the stepwise regression is *k_lith*, the tangential fracture permeability in lithophysal units. The R-square improves from 28% to 44% with the addition of this seepage parameter. Its sign is negative, as expected (see Sections 4.2 and 4.4).

The third parameter to enter the stepwise regression is *GWSPD*, the ground-water specific discharge multiplier. The R-square improves from 44% to 58% with the addition of this ground-water flow parameter. Its sign is positive, indicating that a change from its mean to a one standard deviation higher value of *GWSPD* leads to a (logged) peak dose forecast that is approximately 0.35 standard deviations above its mean forecasted peak dose.

The fourth parameter to enter the regression is *Repos_Avg_Infil_LTA*, the repository long-term average infiltration rate. The R-square improves from 58% to 67% with the addition of this parameter. Its sign is again positive, as expected (see Section 4.4). The fifth parameter to enter is *one_over_alpha_A*, the capillary strength ($1/\alpha$) above the drift. The R-square improves from 67% to 70% with the addition of this seepage parameter. Its sign is negative, as expected (see Sections 4.3 and 4.4).

¹⁵ This parameter is used to capture uncertainty in the ground-water specific discharge from the saturated zone. The parameter is a multiplication factor that is applied to all values of permeability and specified ground-water fluxes to scale the simulated discharge in the SZ transport module.

Table 13. Characteristics of the 22 Parameters Selected by Stepwise Regression Procedure Applied to Run 1
(Source: Run 1)

Rank	Parameter_Name	Parameter_Description	GoldSim Module	Type Distribution	Mean	StdDev	Min	Max
1	<i>Log_Pu_Sol_eps1</i>	Uncertainty in solubility thermodynamics (Pu)	\Source_Term_Models	TruncNormal	0	1	-2	2
2	<i>k_lith</i>	Fracture permeability (lithophysal units)	\Drift_Seepage_Model	Triangular	-11.5	0.37559	-12.42	-10.58
3	<i>GWSPD</i>	Ground-water specific discharge multiplier	\Saturated_Zone	ECDF	-0.02385	0.4698	-1.477	1
4	<i>Repos_Avg_Infil_LTA</i>	Repository long term average infiltration rate	\Infiltration_Model	Discrete	29.414	15.2445	1	3
5	<i>one_over_alpha_A</i>	Capillary strength above drift	\Drift_Seepage_Model	Triangular	591	42.866	486	696
6	<i>Pu239_BDCF</i>	Biosphere dose conversion factor (Pu239)	\Biosphere	ECDF	5.24E-03	3.33E-03	1.20E-03	2.17E-02
7	<i>HAVO</i>	Ratio of horizontal anisotropy in permeability	\Saturated_Zone	ECDF	5.6048	4.4497	0.05	20
8	<i>Kd_Pu_FeOx_CP</i>	Distribution coefficient in corrosion product (Pu)	\Source_Term_Models	LogUniform	1252.5	1274.8	100	5000
9	<i>NVF19</i>	Effective porosity in shallow alluvium	\Saturated_Zone	TruncNormal	0.18	0.051	0	0.3
10	<i>Tc99_BDCF</i>	Biosphere dose conversion factor (Tc99)	\Biosphere	ECDF	5.22E-06	1.12E-05	1.87E-06	8.96E-05
11	<i>Flow_Focusing_Factor</i>	Seepage flow focusing factor	\Drift_Seepage_Model	Uniform	1.5	0.28868	1	2
12	<i>FPLAW</i>	Western boundary of alluvial uncertainty zone	\Saturated_Zone	Uniform	0.5	0.28868	0	1
13	<i>Pu242_BDCF</i>	Biosphere dose conversion factor (Pu242)	\Biosphere	ECDF	4.91E-03	3.15E-03	1.13E-03	2.05E-02
14	<i>Log_Np_Sol_eps1_NpO2</i>	Uncertainty in solubility thermodynamics (NpO ₂)	\Source_Term_Models	TruncNormal	0	0.6	-1.2	1.2
15	<i>Kd_Pu_Al</i>	Distribution coefficient in the alluvium (Pu)	\Saturated_Zone	Beta	100	15	50	300
16	<i>k_nonlith</i>	Fracture permeability (non-lithophysal units)	\Drift_Seepage_Model	Triangular	-12.2	0.27761	-12.88	-11.52
17	<i>HLW_Inventory_Unct</i>	High-level waste inventory uncertainty	\Source_Term_Models	Triangular	1.0667	0.16499	0.7	1.5
18	<i>Np237_BDCF</i>	Biosphere dose conversion factor (Np237)	\Biosphere	ECDF	1.17E-03	8.28E-04	3.61E-04	5.54E-03
19	<i>pH_CDSP_High_Q</i>	CDSP In-package pH (high flow rate)	\Source_Term_Models	Uniform	6.25	1.0104	4.5	8
20	<i>Th230_BDCF</i>	Biosphere dose conversion factor (Th230)	\Biosphere	ECDF	1.50E-02	1.27E-02	1.03E-03	7.07E-02
21	<i>U233_BDCF</i>	Biosphere dose conversion factor (U233)	\Biosphere	ECDF	6.13E-04	7.75E-04	1.48E-04	5.16E-03
22	<i>Kd_Th_Invert</i>	Distribution coefficient in the invert (Th)	\Source_Term_Models	Uniform	5500	2598.1	1000	10000

Table 14. Coefficients and Statistics for Parameters Accepted in Stepwise Regression of Annual Dose Maxima versus All 76 Stochastic Parameters Used in EPA Uncertainty Model
(N=1000 realizations, R² = 0.801) (Source: Run 1)

ID	Model Parameters in Order of Entry into SPSS Stepwise Regression Procedure	Unstandardized Coefficients ^a		Standardized Coefficients ^a	t-Statistic	Sig.	95% Confidence Interval for B		R Square	Adjusted R Square	R Square Change
		B	Std. Error	Beta			Lower Bound	Upper Bound			
0	Constant	-10.138	0.730		-13.882	0.000	-11.572	-8.705			
1	Log_Pu_Sol_eps1	0.533	0.015	0.529	36.708	0.000	0.504	0.561	0.283	0.283	0.283
2	k_lith	-0.981	0.034	-0.415	-28.752	0.000	-1.048	-0.914	0.436	0.435	0.152
3	GWSPD	0.667	0.027	0.354	24.523	0.000	0.614	0.721	0.580	0.578	0.144
4	Repos_Avg_Infil_LTA	0.019	0.001	0.320	22.176	0.000	0.017	0.020	0.673	0.672	0.093
5	one_over_alpha_A	-0.004	0.000	-0.169	-11.776	0.000	-0.004	-0.003	0.705	0.704	0.032
6	Pu239_BDCF	33.986	3.834	0.128	8.865	0.000	26.462	41.509	0.724	0.722	0.018
7	HAVO	0.023	0.003	0.118	8.182	0.000	0.018	0.029	0.738	0.737	0.015
8	Kd_Pu_FeOx_CP	-7.80E-05	1.01E-05	-0.112	-7.745	0.000	-9.77E-05	-5.82E-05	0.749	0.747	0.011
9	NVF19	-1.779	0.260	-0.099	-6.854	0.000	-2.288	-1.270	0.758	0.756	0.009
10	Tc99_BDCF	6,056.524	1,140.710	0.077	5.309	0.000	3,818.000	8,295.047	0.765	0.763	0.007
11	Flow_Focusing_Factor	0.273	0.044	0.089	6.188	0.000	0.187	0.360	0.772	0.770	0.007
12	FPLAW	-0.223	0.044	-0.073	-5.063	0.000	-0.310	-0.137	0.778	0.775	0.006
13	Pu242_BDCF	18.626	4.062	0.066	4.585	0.000	10.653	26.598	0.782	0.780	0.004
14	Log_Np_Sol_eps1_NpO2	0.108	0.024	0.065	4.487	0.000	0.061	0.156	0.787	0.784	0.004
15	Kd_Pu_Al	-0.003	0.001	-0.055	-3.771	0.000	-0.005	-0.002	0.790	0.786	0.003
16	k_nonlith	-0.166	0.046	-0.052	-3.604	0.000	-0.256	-0.075	0.792	0.789	0.003
17	HLW_Inventory_Unct	0.240	0.078	0.045	3.094	0.002	0.088	0.392	0.794	0.791	0.002
18	Np237_BDCF	42.713	15.461	0.040	2.763	0.006	12.372	73.054	0.796	0.792	0.002
19	pH_CDSP_High_Q	-0.035	0.013	-0.040	-2.784	0.005	-0.060	-0.010	0.797	0.793	0.002
20	Th230_BDCF	2.800	1.001	0.040	2.797	0.005	0.835	4.764	0.799	0.795	0.001
21	U233_BDCF	39.396	16.526	0.034	2.384	0.017	6.967	71.826	0.800	0.796	0.001
22	Kd_Th_Invert	1.14E-05	4.91E-06	0.034	2.328	0.020	1.80E-06	2.11E-05	0.801	0.797	0.001

a Dependent Variable: Log10_Maximum_Dose

The next five parameters (ranks 6 through 10) in Table 14 include two more sources of uncertainty concerning plutonium—the BDCF for Pu-239 (*Pu239_BDCF*) and the k_d coefficient for Pu in corrosion products (*Kd_Pu_FeOx_CP*), two additional ground-water flow parameters—the ratio of horizontal anisotropy in permeability (*HAVO*) and the effective porosity in the shallow alluvium (*NVF19*), and the BDCF for Tc-99 (*Tc99_BDCF*) which is an important contributor to the total annual dose in the EPA Uncertainty Model. The parameters in ranks 11 through 15 in Table 14 include the familiar seepage flow focusing factor from Section 4.2, two additional sources of uncertainty concerning plutonium—the BDCF for Pu-242 (*Pu242_BDCF*) and the k_d coefficient for Pu in the alluvium (*Kd_Pu_Al*), the uncertainty in NpO_2 solubility thermodynamics (*Log_Np_Sol_eps1_NpO2*), and an additional ground-water flow parameter (*FPLAW*), which marks the western boundary of the alluvial uncertainty zone, reflecting uncertainty concerning its length.

The relative magnitude and direction of the estimated standardized coefficients for the 22 parameters selected in the stepwise regression are shown in Figure 22. Given the selection of these 22 parameters by the stepwise regression process, the remaining 54 have no additional explanatory power (see Appendix B, Table B-4). The relatively larger sizes of the standardized coefficients for the first five parameters selected in the stepwise regression are shown by the three bars at the top of the figure and the two bars at the bottom. All 54 unselected model parameters listed in Appendix B, Table B-4, will have smaller influence on the forecasted peak dose than the 22 selected parameters shown in this figure, and would fall on the plot between the smallest positive bar (*Kd_Th_Invert*) and the least negative bar (*pH_CDSP_High_Q*).

One measure of the relative importance of the variables in the stepwise regression analysis of all model parameters is the increase in R-square obtained as the selected parameters are added stepwise to the regression model. The increase in R-square for each added variable is shown in the right-hand column of Table 14. Figure 23 shows the 22 selected model parameters ranked by the increase in R-square obtained when added to the regression model. Parameter descriptions are used in this figure to provide more information on the role of each of these important model parameters. The increase in R-square decreases as additional variables enter the regression. Hence, the order of parameters in this figure is the same as discussed for Table 14.

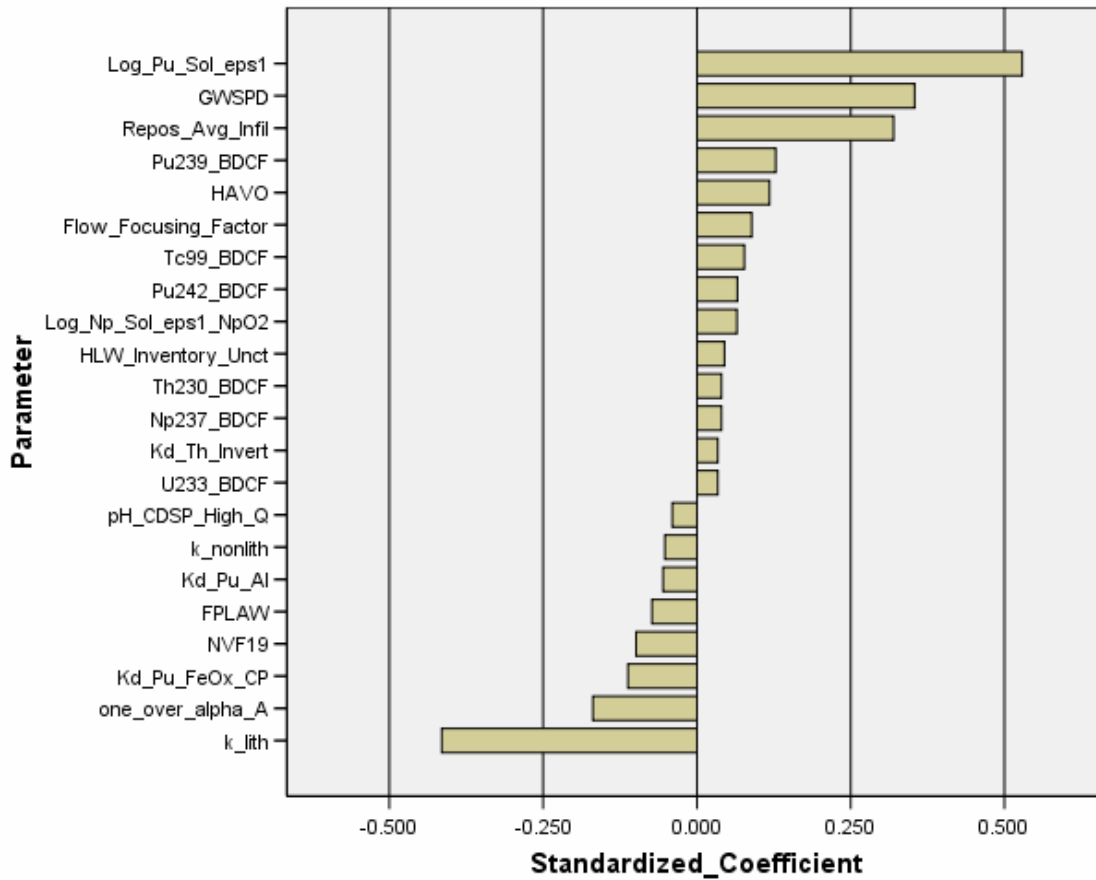


Figure 22. Standardized Coefficients of 22 Most Significant Parameters in Stepwise Regression of Annual Dose Maxima versus All 76 Stochastic Parameters used in EPA Uncertainty Model
 (N=1000 realizations, $R^2 = 0.801$) (Source: Run 1)

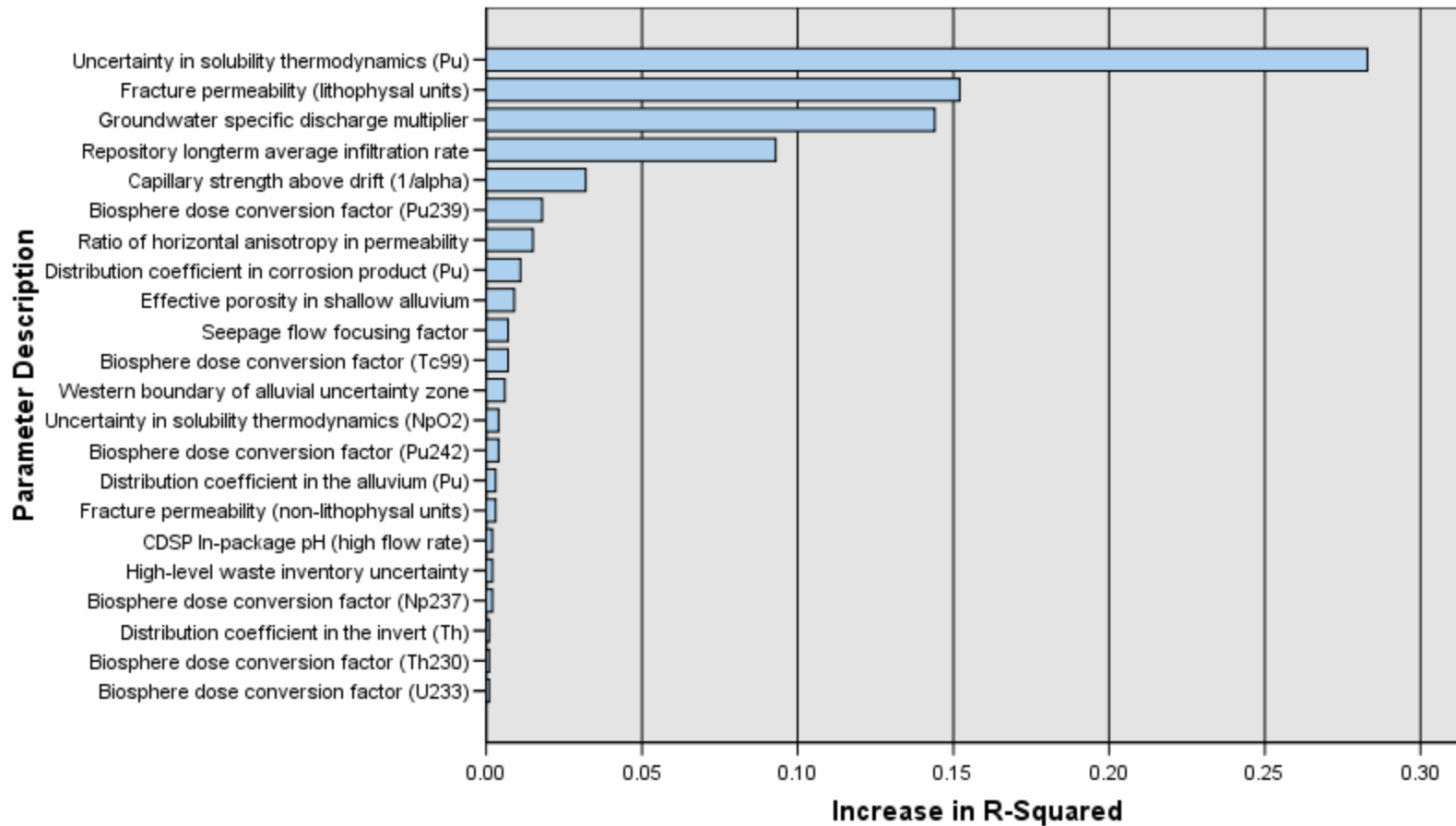


Figure 23. Increase in R-Squared Achieved by Stepwise Addition of the 22 Selected Parameters in Regression of Annual Dose Maxima versus All 76 Stochastic Parameters Used in EPA Uncertainty Model
 (N=1000 realizations, $R^2 = 0.801$) (Source: Run 1)

5.0 IMPLICATIONS OF RESULTS FOR STANDARDS SETTING

5.1 CHARACTERIZATION OF EPA UNCERTAINTY MODEL

The EPA Uncertainty Model is not a predictor of the actual expected performance of the Yucca Mountain disposal system. Rather, it is a model designed to show how a hypothetical disposal system that operates at the edge of compliance at 10,000 years, delivering a mean dose to the RMEI of 15 mrem/yr, will continue to perform over longer times within the period of geologic stability. The analyses presented here illustrate the sensitivity of this longer-term performance to important parameters related to natural barriers and radionuclide solubilities. The effects of selected features of the engineered barriers (drip shields and some waste packages) on long-term doses are removed in the EPA model.

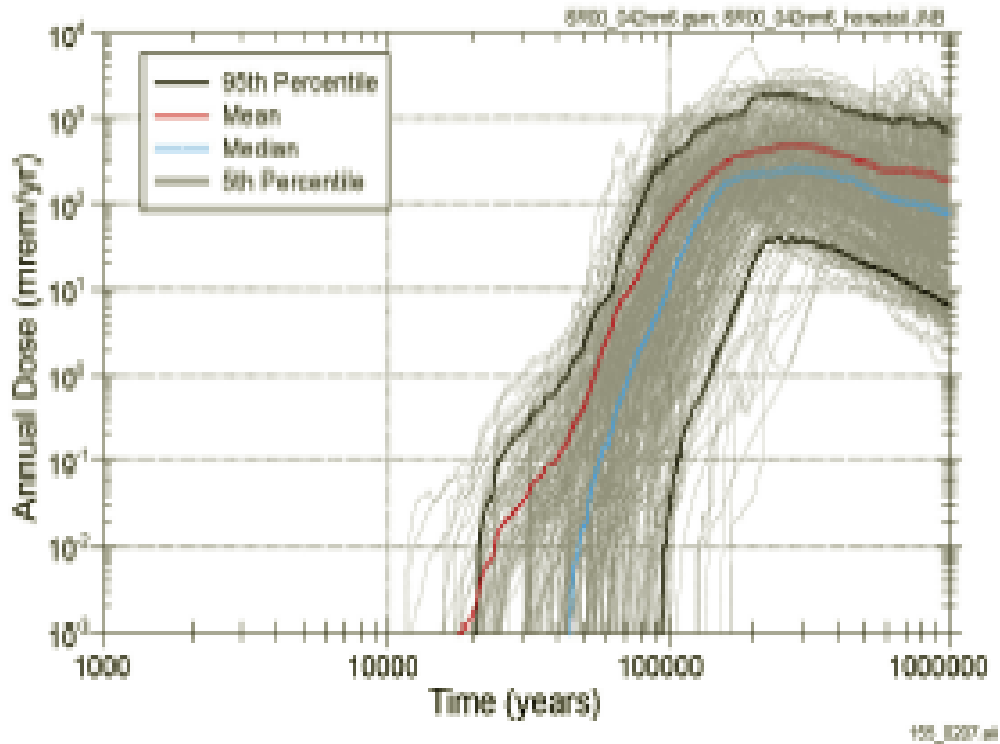
The performance of the hypothetical system examined here should not be taken as a reflection of the actual performance of the Yucca Mountain disposal system being developed by DOE. The behavior of the actual disposal system will depend strongly on the corrosion resistance behavior of the EBS components (OCRWM 2005), since the engineered barriers are a major factor in controlling radionuclide releases over long periods of time. Without an early failure mechanism, waste packages may not begin failing by general corrosion for several hundred thousand years. However, it must be remembered that the DOE Peak Dose Model upon which the EPA Uncertainty Model is based contains many simplifications and abstractions of the more complex models used by DOE in a full TSPA. Some of these simplifications and abstractions could understate performance based on a full set of models.

5.2 DOE LONG-TERM PROJECTIONS OF SITE PERFORMANCE

This section describes several projections made by DOE of the performance of the Yucca Mountain repository beyond 10,000 years, but within the period of geologic stability. Generally, these were complete performance assessments for the entire repository system using the full range of models available at the time they were performed. Additional descriptions of these performance assessments may be found in the Background Information Document of the proposed revisions to 40 CFR 197 (EPA 2005, Section 12) and/or in the DOE reports referenced below. These full performance assessment results provide a qualitative basis for comparison with the simplified models discussed previously in Sections 2, 3, and 4. These models demonstrate increasing uncertainty up to the time of the peak dose. They also indicate considerable variability in the magnitude of the peak dose based on selected modeling assumptions within the range of reasonable options.

5.2.1 Total System Performance Assessment for the Site Recommendation

In the 2000 TSPA-SR, the modeling approach used by DOE resulted in no waste package failures and, consequently, no doses during the first 10,000 years (CRWMS M&O 2000, Figure 4.1-5). Extending the TSPA-SR models to 1,000,000 years with no modification resulted in a mean peak dose of 490 mrem/yr at 270,000 years. The primary contributor to peak dose is Np-237, with smaller contributions from colloids on Th, Ra, and Pu (CRWMS M&O 2000, Section 4.1.3). Results for this modeling case are presented in Figure 24.



155_0007.ai

Source: TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Figure 4.1-19a).

Figure 24. Simulated Annual Dose Histories for the Total System Performance Assessment for Site Recommendation Nominal Case
(CRWMS M&O 2000, Figure 4.1-19a)

DOE also examined an alternative modeling approach, where they assumed that neptunium was incorporated as a solid solution into a secondary uranium mineral formed by reaction of the uranium dioxide fuel with water. In this model, the Np-237 solubility was substantially reduced. For this alternative scenario, the mean peak dose was about 30 mrem/yr occurring at about 1,000,000 years (CRWMS M&O 2000, Section 4.1.3).

DOE also considered another alternative long-term TSPA-SR model, where glacial climates were assumed to recur several times over a 1,000,000-year period, significantly altering infiltration rates. In this alternative model, the secondary phase solubility approach was retained. The incorporation of the glacial climates caused the mean peak dose to increase to 120 mrem/yr from 30 mrem/yr with unaltered long-term climate and the time of the mean peak dose to decrease to 700,000 years (CRWMS M&O 2000, Section 4.1.3).

5.2.2 Supplemental Science and Performance Analyses

In the 2001 Supplemental Science and Performance Analyses (SSPA), the modeling retained features of the alternative TSPA-SR long-term models, including incorporation of recurring glacial climates and actinide solubilities limited by dissolution of secondary uranium minerals. A major modification made to the SSPA model was the assumption of temperature dependency of the general corrosion rate for the Alloy 22 used in the waste package outer container. In the SSPA, the general corrosion rate was assumed to decrease with decreasing temperature based on an Arrhenius relationship. The SSPA includes limited early waste package failures caused by improper heat treatment of closure welds. All model changes are summarized in Section 4.1 of BSC 2001. A comparison of results for the SSPA modeling with the TSPA-SR results is presented in Figure 25. The *base case* curve shown in this figure is the same as the mean dose curve in Figure 24 for the TSPA-SR nominal case. SSPA results are shown for both the higher-temperature operating mode (HTOM) and the lower-temperature operating mode (LTOM). The HTOM is based on a thermal-hydrologic model similar to that used in the TSPA-SR. The LTOM uses a reduced areal loading of waste packages in the repository to reduce the influence of heat effects from radioactive decay.

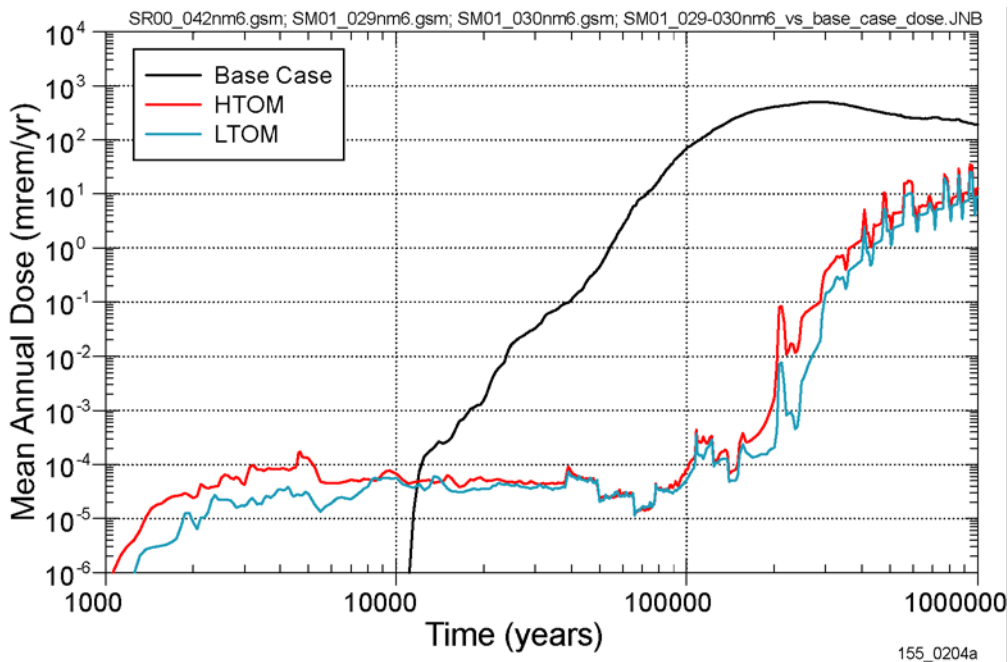


Figure 25. One Million-Year Dose Histories for Supplemental Science and Performance Analyses Higher-Temperature Operating Mode and Lower-Temperature Operating Mode Models Compared to Total System Performance Assessment for Site Recommendation Nominal Case

(BSC 2001, Figure 4.1-1)

The mean dose in the SSPA models is about 35 mrem/yr at 1,000,000 years and is continuing to increase at a low rate. The mean dose of 35 mrem/yr as compared to a mean peak dose of 120 mrem/yr for the TSPA-SR alternative model demonstrates the importance of assuming that the waste package general corrosion rate is temperature dependent.

5.2.3 Revised Supplemental Total System Performance Assessment

The Revised Supplemental TSPA was used by DOE to provide input to the 2002 Final Environmental Impact Statement (FEIS). The performance of the repository based on this revised performance assessment is shown here in Figure 26 (OCRWM 2002a, Figure I-12). The figure shows the annual dose to the RMEI for the HTOM that includes a thermal-hydrologic model similar to that used in the TSPA-SR. In this model, a limited number of early failures of waste packages (0 to 5) are assumed to occur due to inadequate heat treatment of closure welds in the Alloy 22 (OCRWM 2002a, Table I-3). This results in a dose at 10,000 years of about 10^{-5} mrem/yr, as contrasted to a value of 15 mrem/yr set as the initial condition in the EPA Uncertainty Model. Temperature dependency of Alloy 22 general corrosion is not included in the model. A peak mean dose of 152.5 mrem/yr is reached at 476,000 years (OCRWM 2002a, Table I-13). The spikes in Figure 26 are due to the assumption of discrete climate (infiltration rate) changes at times listed in Table 1 of OCRWM 2005. These climate spikes were eliminated by using long-term weighted averages for infiltration rates in the DOE Peak Dose Model and the EPA Uncertainty Model.

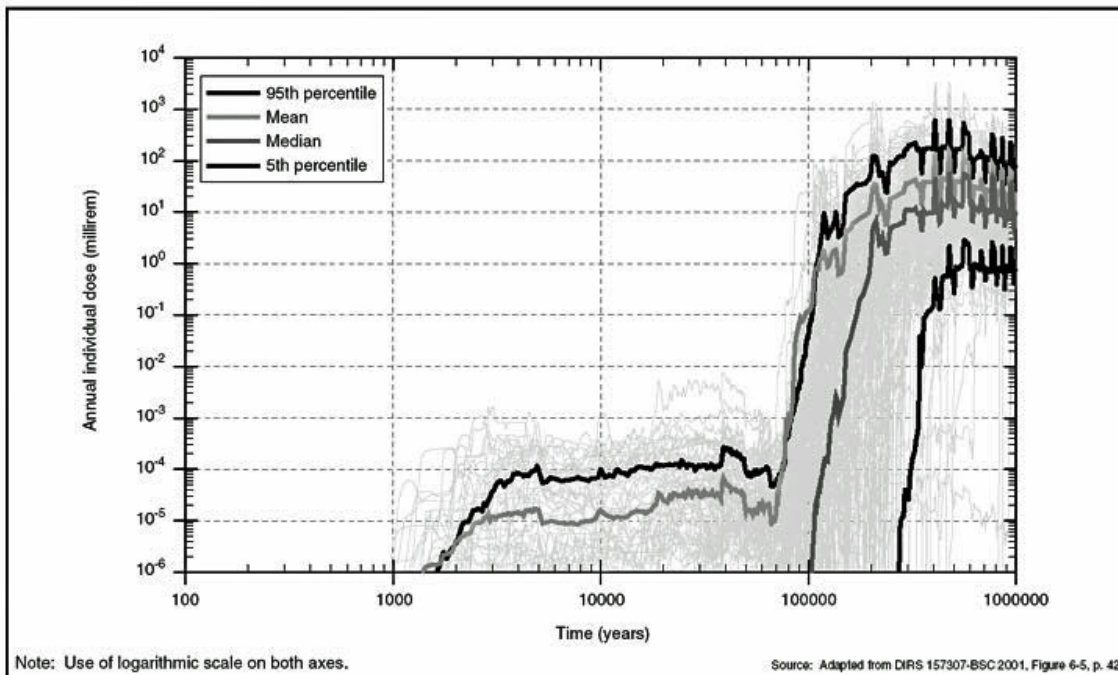


Figure 26. Revised Supplemental Total System Performance Assessment 1,000,000-Year Dose Histories Based on Final Environmental Impact Statement Higher-Temperature Operating Mode

(Source: OCRWM 2002a, Figure I-12)

Results of these long-term DOE performance assessments are summarized in Table 15.

Table 15. Summary of Results for Long-Term DOE Yucca Mountain Performance Assessments

Performance Assessment Model ^a	Mean Peak Dose (mrem/yr)	Time of Peak Dose (years)	Important Contributors to Dose
TSPA-SR nominal	490	270,000	Np-237 (dominant), colloids of Th, Ra, and Pu
TSPA-SR w/ modified solubilities	30	About 1,000,000	Pu-242, Pa-231
TSPA-SR w/ modified solubilities and recurring glacial climates	120	700,000	N/A ^c
SSPA (modified solubilities, recurring glacial climates and temperature-dependent Alloy 22 corrosion)	35 ^b	>1 million	Np-237, Pa-231
FEIS (similar to SSPA but w/ temperature independent Alloy 22 corrosion)	152.5	476,000	N/A
DOE Peak Dose Model	125	730,000	Pu-242, Np-237

a – Model descriptions are intended to indicate most important features and not all changes from model to model

b - Mean dose at 1,000,000 years; dose continues to increase beyond 1,000,000 years

c – N/A: not available in references cited in Section 5.2

The various DOE long-term performance assessment models used in the TSPA-SR, the SSPA, the FEIS, and the Peak Dose Model generated mean peak doses ranging from 30 to 490 mrem/yr with the time of peak dose ranging from 270,000 years to more than 1,000,000 years. Significant releases from early failures did not occur in any of these models due to the robust nature of the engineered barriers. It should be noted that all these performance assessments, except for the DOE Peak Dose Model, were based on BDCFs from ICRP 30. The BDCFs in the DOE Peak Dose Model are based on ICRP 72. The more recent BDCFs are approximately a factor of 4 lower, which means that the results for the various TSPAs should be reduced accordingly (OCWRM 2002b, Section 5.4.2.3).

5.2.4 Uncertainty in DOE and EPA Modeling Projections

It is not possible to directly compare the dose level projections and peak dose time results from the EPA Uncertainty Model with the results of DOE's previous modeling of the actual Yucca Mountain disposal system. This is because the EPA modeling involves a hypothetical disposal system constructed to be deliberately at "the edge-of-compliance" at 10,000 years, whereas the DOE modeling was performed to assess performance of the actual disposal system starting initially from total containment. In the EPA uncertainty modeling, a deliberately failed EBS system was created to set a base case (which included uncertainty in the site conditions to derive a mean dose at 10,000 years with an associated uncertainty), against which the propagation of uncertainty in the long term could be examined. The EBS performance was held constant, essentially to look at the effects of uncertainty in natural barrier performance on the dose projections over time from a fixed repository source term. In contrast, the DOE modeling is

designed to examine the entire disposal system performance from repository closure, and considers the integrated performance of the engineered and natural barriers.

However, some comparisons against the DOE assessments can be made with respect to the projected performance of the natural barrier system in the long-term, i.e., after a point in time where the EBS can be assumed to have limited containment capability and functions largely as a source term for releases in the repository into the intruding ground water. The areas where the respective modeling results can be compared are the dose histories after the peak dose time in the DOE assessments and the peak dose area for the EPA uncertainty analyses. In the post-peak dose portion of the DOE assessments, the EBS is effectively functioning as a source term for far-field transport since at these times the EBS has lost its major containment role.

The results discussed in Section 3.2 point to an uncertainty increase of approximately two orders of magnitude between the EPA reference system at 10,000 years and that at peak dose. This represents the uncertainty in the natural barrier as it influences the peak dose from the hypothetical “edge-of-compliance” disposal system used as the starting point. DOE’s assessments indicate that the travel time and flow rates through the repository are sufficient to “flush” the contents of failed packages quickly from the EBS and into the natural barrier (OCRWM 2005). The relatively quick ground-water travel time from the repository to the receptor (on the order of thousands of years) and the long time frame for the assessments indicates that the behavior of the dose history curves reflect the behavior of the EBS over the long time span and the effects of the natural barrier to limit releases from the repository (through limited ground-water access, solubility constraints, and far-field retardation processes). The long-term interplay of EBS degradation and natural barrier attenuation can be seen in Figure 24 (from the TSPA-SR analysis) and Figure 26 (from the DOE FEIS analyses). Other comparable examples include different models from the SSPA, such as those illustrated in Figure 4.2.5.5 of BSC 2001. All of these figures show approximately a two order of magnitude spread between the 5th and 95th percentile of the dose distribution in the region beyond the peak dose, a spread similar to that observed with the EPA Uncertainty Model between the Baseline at 10,000 years and the time of the peak dose. The maximum uncertainty in the DOE projections (reflected in the spread between the 5th and 95th percentiles) occurs when the dose curves are rising steeply. This is reflective of the time period when the EBS portion of the disposal system is actively degrading and releasing radionuclides to the natural barrier. At later times, these portions of the DOE dose projections represent the situation when the EBS system has broken down significantly and is functioning as a relatively constant source term release to the natural barrier (a gradual decline in the long-term projections would reflect a diminishing source term due to decay of the long-lived inventory in the repository). In the post-peak region of the DOE projections, failure of additional waste packages would contribute to the dose levels quickly, reflecting the ground-water travel time estimates for transport through the natural barrier, and the projected dose history strongly reflects the performance of the natural barrier.

The interesting result of the comparison of EPA and DOE modeling is what it reveals about the ability of the dose projection methodology to distinguish between alternate conceptualizations of the disposal system performance. Each of the DOE assessments reported is an alternative conceptual model of the disposal system, with differing assumptions about the repository configuration and performance of the natural and engineered barriers over time. Likewise the

EPA uncertainty modeling is also based on a different conceptual model than used in the DOE performance modeling. In the case of the EPA uncertainty modeling, the conceptualization of the disposal system performance is a more simplified construct of the actual disposal system functions. One should remember that the EPA Uncertainty Model was based on the DOE Peak Dose Model, which removed elements from the actual repository design that were believed to contribute little to the eventual peak dose but retained elements that had meaningful contributions to the peak dose projections. In the DOE performance assessment models, the post-peak portion of the disposal histories reflects the time when the EBS has lost much of its containment capability and is functioning as a generally constant source term for releases to the natural barriers, i.e., the EBS is largely removed from the system. The EPA Uncertainty Model removes the EBS containment initially and reflects the behavior of the natural barriers throughout the modeling period.

The point of comparison for uncertainty in the natural barrier performance is the post-peak dose portion of the DOE dose histories and the peak dose in the EPA uncertainty modeling. Both the DOE and EPA modeling show approximately two orders of magnitude in the variation of dose projections. This suggests strongly that this estimate of uncertainty (about two orders of magnitude) could be regarded as the practical limit of the modeling to distinguish between performance projections of alternate conceptual models of the disposal system when the EBS has ceased to provide a high degree of containment for the radionuclides within the repository. This limit on meaningful projections of performance over very long time frames on the order of hundreds of thousands of years supports the general position that repository performance projections become less “confident” in these time periods. Their ability to meaningfully distinguish between alternate conceptualizations of the disposal system decreases significantly.

5.3 SUMMARY OF EPA MODELING RESULTS

In comparison to the DOE results discussed in Section 5.2, the EPA Uncertainty Model was set to produce a mean peak dose of 15 mrem/yr at 10,000 years by severely limiting the performance of the EBS. The estimated mean peak dose from the early waste package failures was 342 mrem/yr. As shown in Table 1, the 95% confidence interval for the estimated mean based on 1,000 realizations extends from 269 to 415 mrem/yr. This indicates approximately a $\pm 20\%$ spread in the peak mean dose estimate based on uncertainty/variability of the input parameters. It should be remembered that this dose does not include any contribution from failures of the remaining waste packages by general corrosion at much later times. General corrosion failures were evaluated in the DOE Peak Dose Model, but not in the EPA Uncertainty Model.

As mentioned earlier, the primary objective of the analyses presented here is to assess the effects of uncertainties over time on the projected location of the “edge of compliance” for the hypothetical disposal system at 10,000 years. As described in Section 2.2.2, the database contained in the DOE Peak Dose Model and used, basically unaltered, in the EPA analyses reflects the variability of repository parameters based on laboratory and field studies. It also contains estimates of uncertainty based on professional judgments of how these parameters may change over the performance period. Results for our assessments for a fixed disposal system configuration at one point in time (10,000 years) offer the possibility of demonstrating how inherent uncertainties in the database and the model evolve over the stability period. As long as

the processes that control the release and transport of radionuclides from the disposal system are kept the same between the reference case construction (determining the number of package failures necessary to create the EPA Baseline at 10,000 years) and the subsequent long-term performance of that same disposal system, the effects of uncertainties in the defined system can be assessed. Uncertainty in the mean dose due to parametric uncertainty/variability increases from about 1.5 orders of magnitude at 10,000 years (based on the spread between the 5th and 95th percentiles) to about 3.5 orders of magnitude at the time of the peak dose (64,000 years) from the early failures. The uncertainty then decreases to about 2 orders of magnitude at about 200,000 years before increasing to about 4.6 orders of magnitude at 1,000,000 years.

An analysis of the mean peak dose as a function of the number of realizations was conducted over the range from 300 to 5,000 realizations (Table 1). The highest value obtained (393 mrem/yr at 5,000 realizations) was 13% higher than the result for 1,000 realizations. A run of 1,000 realizations with the Latin Hypercube Sampling (LHS) option removed showed a peak dose of 408 mrem/yr (Table 2). This peak dose was 19% higher than the peak dose for 1,000 realizations using the LHS option. However, all peak dose estimates from random parameter runs in Tables 1 and 2 fell within the 95% confidence interval for the estimated mean peak dose based on 1,000 realizations using the LHS option.

From these results, it is evident that uncertainties reflected in the database result in wide variations in estimates of the mean of the peak dose projections, and support the somewhat intuitive expectation that uncertainties would increase over long time frames.

The median dose is generally significantly lower than the arithmetic mean dose. For example, when the mean dose at 10,000 years calculated with the EPA Uncertainty Model is set at 15 mrem/yr by fixing the number of waste package failures at 520 and allowing all other parameters to vary, the equivalent median dose is 3 mrem/yr. The median peak dose of 26.6 mrem/yr occurs at 112,000 years. This estimate of the median remains stable when a higher number of realizations are generated.

The mean peak dose is skewed toward the upper limits of the distribution of realizations, as demonstrated by the fact that 84% of the realizations have values that are less than the mean peak value of 342 mrem/yr. In contrast, there are 228 (22.8%) realizations with a peak annual dose less than 15 mrem/yr.

Realizations with double peaks are common. A “deep valley” pattern occurs in a small fraction of the realizations. A “valley” is formed at the time of the peak dose due to complete removal of Tc-99 before that time in some realizations. Eventually, other slower-moving species reach the receptor location, creating a second peak in the total dose. In general, the double top pattern is due to the separation of the fast- and slow-moving radionuclides, given the finite masses in the source term.

A detailed stepwise regression analysis of all variable parameters in the EPA Uncertainty Model shows that the most important parameter contributing to variability in the mean peak dose is uncertainty in the thermodynamic properties used to model Pu solubility (*Log_Pu_Sol_eps1*). This parameter accounts for 28% of the total variability. The four next most important

parameters (in descending order) are tangential fracture permeability of the lithophysal units (*k_{lith}*), ground-water specific discharge multiplier (*GWSPD*), repository long-term average repository infiltration rate (*Repos_Avg_Infil_LTA*), and capillary strength in fractured rock in drift crown (*one_over_alpha_A*). Together, these five parameters account for about 71% of the total variability in the peak dose.

5.4 EFFECT OF CONSERVATIVE ASSUMPTIONS IN THE MODELING

The DOE Peak Dose Model is based on abstractions designed for eventual use in TSPA models that will be used for license application compliance assessments. In DOE's documentation for the Peak Dose Model, there are numerous references to conservative assumptions built into the model (for example, deletion of the UZ and a portion of the SZ from the travel path for releases). In developing the EPA Uncertainty Model, these conservative assumptions were simply carried into the EPA model. In using the results of the EPA model calculations to assess what potential peak doses could be produced from the 10,000-year "edge of compliance," there could be a question about the effects of the conservative assumptions in the DOE Peak Dose Model (where conservatism means assumptions that tend to overestimate doses relative to less conservative, i.e., more realistic, assumptions). Are the results of the calculations presented in this report biased toward much larger doses than would truly be expected for the hypothetical disposal system at the "edge of compliance" at 10,000 years? This should not be of concern, as the focus in these analyses on the relationship between projected doses and their evolution over time, rather than on the absolute values of individual scenarios examined in our studies. The analyses presented here are essentially comparative in nature, in that a hypothetical disposal system was created using the DOE model, with its built-in conservatisms, and then the peak dose projections made relative to that hypothetical starting point. In essence, the conservatisms in estimating releases tend to counterbalance each other when comparing respective outputs. A model using different assumptions would result in a different number of waste packages failures to produce the 15 mrem/yr dose at 10,000 years. It is not possible to quantitatively assess the relative effects of differing possible conservative assumptions on these analyses without a more complex site model. Since the analyses presented here are comparative, the inherent conservatisms in the models should not bias the results, as long as there are no changes in the model structure and assumptions between the calculations used to set up the 10,000-year disposal system and the calculations to assess the range of peak dose estimates (for example, see discussion of increased SZ length in Section 3.2).

It is important to note that in doing the analyses with the EPA Uncertainty Model, there was no manipulation of the site database contained in the DOE Peak Dose Model. The data used in the DOE model were derived from the extensive site and laboratory investigations conducted by the DOE since site characterization efforts were initiated in 1988. DOE will also use these data in performing the TSPA compliance modeling that will be submitted to the NRC. The DOE Peak Dose Model is exhaustively documented as to the sources of the data used in the model and the references to these sources. In addition, the changes made to the DOE model to develop the EPA Uncertainty Model are documented in appendices to this report and the Quality Assurance report, which accompanies this report. The Quality Assurance report documents the testing done to verify that the changes made to the DOE model perform as intended, and the independent reviews demonstrate the quality of the work.

5.5 IMPLICATIONS FOR SETTING A PEAK DOSE STANDARD

Many comments received by the Agency on the draft Yucca Mountain standards were concerned with the perceived “loosening” of the peak dose standard because the proposed limit was higher than the 15 mrem/yr mean dose limit established in 40 CFR Part 191 and the 2001 standards. Commenters further stated that uncertainties in dose projections over different time frames alone did not justify higher dose limits at later times. Other commenters voiced opinions on the “protectiveness” of the proposed peak dose limit of 350 mrem/yr. The analyses presented here were performed to address these criticisms and provide some insight on long-term dose projections.

As discussed in Section 1 of this report, the Part 191 standards were established for only the initial 10,000 years of what was envisioned to constitute permanent disposal of these wastes. The 10,000-year limit was predicated on the assumption that projecting doses beyond that time period would be too uncertain for reliable regulatory decision-making. There was no assumption that releases would, or could, be limited to that level for all time by the natural barrier after the engineered barrier could no longer be assumed to provide containment. Rather, the functions of the natural barrier are to create stable conditions for the engineered barrier to maintain its containment function for as long as practicable, and, after the engineered barrier loses its containment function, to keep eventual releases of radionuclides to acceptable levels.

Contrary to this earlier framing of a 10,000-year compliance period in Part 191, the NAS noted that the projected long life of the waste containers in the Yucca Mountain disposal system results in releases largely initiating beyond 10,000 years, as reflected in performance assessments showing peak risks in that time frame (NAS 1995, p.2). The NAS recommended that a standard should be framed to address the time of peak risk, rather than truncated prematurely. While acknowledging uncertainties in dose projections, they also concluded that long time-frame projections of repository performance were possible, and that the performance assessment technology was sufficiently developed to permit projections within a geologic stability period on the order of 1,000,000 years. In response to the 2004 Court decision, the Agency proposed, in 2005, standards for peak dose during this stability period. The results of the analyses presented here shed some light on the quantitative propagation of uncertainty in natural barrier performance over the stability period and have some implications for peak dose standards.

To quantitatively assess the propagation of uncertainty, the modeling set up an “edge-of-compliance” disposal system at 10,000 years and modeled the change in dose projections at peak dose, as detailed in previous sections of this report. The edge-of-compliance case¹⁶ contained a level of uncertainty as a starting point for comparison to the peak dose results. This initial uncertainty was defined by the variations of the input data for the 10,000-year period, as reflected in the variability of the model parameters. These data were contained in the DOE Peak Dose Model database, which in turn were derived through extensive site characterization at

¹⁶ As discussed in Section 3.3, the “edge-of-compliance” case assumes that 520 waste packages fail at random times from 0 to 5,000 years and that all the other parameters are allowed to vary over their assigned uncertainty ranges, resulting in a mean dose to the RMEI of 15 mrem/yr at 10,000 years.

Yucca Mountain. At peak dose, the spread of dose assessments increased by approximately two orders of magnitude from that observed at the initial 10,000 years starting point for the EPA reference system. These results show that uncertainties do in fact increase over the stability period. This uncertainty reflects the natural barrier performance, since the number of failed waste packages used to define the EPA edge-of-compliance case was held constant as a source term (modified through time by decay of the inventory) for releases into the natural barrier. The use of the edge-of-compliance case and the elimination of any additional contribution from the remainder of the waste packages over the simulation period allows the performance of the natural barrier to be examined without confounding variables from additional waste package failures. These results, which demonstrate increasing temporal uncertainty, support the widely voiced assumption that numerical performance projections become less reliable as confident predictors of repository performance over very long time frames. Comparison with DOE dose projections made in Section 5.2.4 suggest that a similar level of uncertainty in dose projections is seen in post-peak dose projections for actual repository designs and performance assessments. The increasing uncertainty in performance projections is a fundamental argument for the selection of background level dose estimates as the peak dose standard as discussed in the 2005 preamble to the proposed standard. The results here support that assumption with a demonstration of uncertainty propagation for the Yucca Mountain site.

The observation that the dose projections for the “edge-of-compliance” case moved from a mean dose of 15 mrem/yr at 10,000 years to mean doses in the range of several hundred millirem/yr depending on the modeling specifics (see Table 10) is notable. The mean dose projections did not remain in the range of only tens of millirems/yr, nor did they move into the area of many thousands of millirem/yr. While it should be recognized that the system we analyzed is hypothetical and actual performance of the Yucca Mountain disposal system will differ, the range of doses for a system set to just meet the 10,000-year standard did not result in dose levels dramatically different than the levels of background doses throughout the United States. These results indicate that the peak dose standard could easily be considered as a level of exposure consistent with a disposal system that would meet the original Part 191 10,000-year standards. From this perspective, the 350 mrem/yr peak dose standard would not be a “loosening” of the original 10,000-year standard, but could be considered as simply a site-specific extension to peak dose over the very long geologic stability period. Actual performance of the Yucca Mountain system will be better or worse than the “edge-of-compliance” case examined here, depending on the actual projections of engineered barrier performance under site conditions. DOE projections of performance are strongly dominated by the corrosion failure rate of the waste packages (OCRWM 2005). If the package failure rate is dramatically faster than DOE projections, the peak dose projections could occur much earlier in time and be higher than current projections indicate. Our assessments attempted to remove this major source of uncertainty from the system by assuming a certain failure rate in the EBS and tailoring the post-10,000-year assessments to evaluate natural barrier performance.

The protectiveness and uncertainty arguments put forward in the 2005 proposal for selecting a background level as the standard are supported by the results of these assessments in that they demonstrate a quantitative increase of uncertainty in the peak dose projections over long time frames. This increasing uncertainty, and corresponding decrease in confidence in long-term dose projections are supportive of the rationale for turning to background levels as acceptable dose

limits in the light of uncertainties in projecting disposal system behavior over very long time frames. The results also lend a degree of confirmatory support to the selection of average background levels as a protective standard, given the uncertainties involved in long-term dose projections.

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APPENDIX A: CODE MODIFICATIONS MADE TO CREATE THE EPA UNCERTAINTY MODEL

GoldSim is an object-oriented simulation code. The code is built using basic “elements” (objects) such as data input elements, function elements, stochastic elements, and graphical output elements. In more traditional code, these elements would be named functions or subroutines. A collection of related elements can be placed in a “container.” A container is similar to a program module that permits localization of the scope of the member elements. The GoldSim code for the Peak Dose Model provided to EPA by DOE was modified by changing existing elements in the code or by adding new elements and containers as required, simulating a hypothetical repository that is on the edge of compliance at 10,000 years. Elements that were newly created elements to develop the EPA Uncertainty Model early failure mode are listed below in Part A. Many of these elements are located in the new *EF_and_Test_Function* container, which holds the input and output elements for the early failure mode. Many other new spreadsheet elements were added to implement the spreadsheet approach for controlling parameters to their mean values. These additional elements are not listed here, but are addressed in a separate QA report. Elements in the original Peak Dose Model code that were modified to create the early failure mode are listed in Part B.

A. New container with test functions and Early Failure (EF) elements

\EF_and_Test_Functions\
New Input Elements

- 1 RunNumber: Type of controlled parameter value to use.¹⁷
- 2 VaryParametersByPercentage: Percent to vary controlled parameters by.
- 3 Total_Number_WPs: Total number WPs in repository (11,184 WPs).
- 4 EF_Mode_Switch: Control for EF mode (0=off, 1=on). Set on Dashboard1.
- 5 EF_Time_Min: First year for early failures.
- 6 EF_Time_Max: Last year for early failures.
- 7 Reference_Dose: Target EF dose (15 mrem/yr at 10,000 yr). Set on Dashboard1.

¹⁷ The following choices are available for RunNumber:

- 0 Use original GoldSim value
- 1 Use mean
- 2 Each parameter independently selected from mean +/-A4%
- 3 All parameters equal vPercent * vMean
- 4 Use median
- 5 Each parameter independently selected from within a CDF range 50% +/-A4%
- 6 All parameters equal the value from the CDF at vPercent
- 7 Select from fixed value set
- 8 Each parameter independently selected with mean +/- A4% * StdDev
- 9 All parameters equal mean + vPercent * StdDev

New Internal Elements

- 1 Design_Early_Failure_Rate: Design fraction of WPs for EF mode.
- 2 Early_Failure_Time: Stochastic. Year of early failure, Uniform(Min, Max).
- 3 EF_Patch_Failures: Complete patch failure by start of next time period.
- 4 Dose_Maximums: Store peak dose and its time for each realization.

New Output Elements

- 1 EF_Percent_WPs_Failed: Percent of WPs for EF mode. Displayed on Dashboard1.
- 2 EF_Total_Number_WPs: Number of WPs selected for EF. Displayed on Dashboard1.
- 3 EF_Dose_History: Annual dose by radionuclide for EF mode.
- 4 EF_Total_Dose_History: Total annual dose for EF mode.
- 5 Maximum_Doses: Save and display peak doses.
- 6 Year_of_Max_Dose: Save and display year of peak dose.
- 7 Waste_Package_EF_History: Save and display patch failure history for EF mode.

B. Modified elements

\Source_Term_Models\Igneous_Intrusion_Model\Igneous_Intrusion\

- 1 Num_WPs_Hit_Ig_Int: Convert to fraction of total number WPs.

\WPandDS_Degradation_Model\Waste_Package_Degradation_Rate\

- 1 Patch_Failures: Correct location of FTD switch in equation.
- 2 Num_CSNF_WPs: Change to controlled fraction of total number of WPs.
- 3 Num_CDSP_WPs: Change to same fraction of total number of WPs as CSNF.
- 4 WP_Initial_Failure_Time_MIC: Insert control for using EF_Failure_Time.
- 5 CSNF_Patch_Failures: Insert control for using EF_Patch_Failures.
- 6 Patch_Failure_Rate: Change percentile from .5 to 5.
- 7 \Full_Temperature_Dependence\Patch_Failure_Rate_FTD: Change percentile from .5 to 5.

\Source_Term_Models\Drift_and_In_Package_Chemistry\

- 1 Starting_Water_Chemistry: Fixed to (3) CS1000 for EF mean or median runs.
- 2 Cracks_Before_Patches: Fixed to .TRUE. for EF mean or median runs.

APPENDIX B: EPA UNCERTAINTY MODEL RUNS AND DESCRIPTION OF PROJECT DISKS

The analyses presented in the main report were derived from a series of 21 runs of the EPA Uncertainty Model. The conditions, assumptions, and check box selections for each model run are presented in Table B-1. The following list describes the characteristics of the runs presented in the fifteen columns of the table. The expanded title of each column is listed in italics. Abbreviations used in the table column headers are indicated in parentheses. Check box and other selections are shown in brackets.

1. *Run Identifier (ID)/Run Name*
2. *Number (#) realizations*
3. *Early failure (EF) mode operational?* [Check box (=Yes)]
4. *Number (#) waste packages (WPs) with early failure*
5. *Time of early failures [yr]*
6. *Drip shield (DS) has no function?* [Check box (=Yes)]
7. *Deterministic infiltration?* [Check box (=Yes)]
8. *Infiltration case* [Check boxes for medium (med), high, and low infiltration]
9. *Vary seepage parameters?* [Y=Yes; N=No]
10. *Vary solubility parameters?* [Y=Yes; N=No]
11. *Vary other parameters?* [Y=Yes; N=No]
12. *I-129 and (&) Tc-99 in inventory?* [Y=Yes; N=No]
13. *Non-collapsed drifts* [Check box (=Yes)]
14. *Saturated zone (SZ) length of 0* [Check box (=Yes)]
15. *RunNumber* [0=All parameters random, unless specified fixed; 1=All parameters fixed, unless specified random]

The number of realizations is set in the GoldSim MODEL|SIMULATION SETTINGS window. Check box selections are made on *Dashboard1*. The number and timing of waste package early failures are set in the *\EF_and_Test_Functions* container. Variation in seepage, solubility and other parameters is controlled by the *SelectValue.xls* spreadsheet found on the same directory or subdirectory as the GoldSim model for each run. Inventories of I-129 and Tc-99 were manually set to 0 in the *\Source_Term_Models\Materials\Inventory* container for runs without these isotopes. The value of the *RunNumber* element controls the mode of operation of the *SelectValue.xls* spreadsheet. The value is set in the *\EF_and_Test_Functions* container.

All check boxes (except the early failure mode check box) previously existed in the DOE Peak Dose Model. The early failure functions in Columns 1, 3 through 5, 9 through 12, and 15 do not exist in the DOE Peak Dose Model.

The location of the GoldSim file for each model run is shown in Table B-2. The directories show the location of each GoldSim file on the project disks. All model runs were made using GoldSim Version 8.02, and are not compatible with other versions of GoldSim. This version of GoldSim is available to registered users from the download page at the GoldSim website. Also listed in Table B-2 are the table, figure and/or section numbers where output from the run is used in the main report.

The 55 model parameters in the All Parameter stepwise regression that were not included in the other sensitivity runs are listed in Table B-3 with their location in the model. The 54 parameters that were not selected in the All Parameter stepwise regression are listed in Table B-4. Also shown are the coefficient estimate, t statistic and significance level for each unselected parameter. Note that all parameters in this table are not statistically significant at the $p=0.05$ level of significance.

The distinguishing features of each model run and its intent in the analysis are described in the following brief summaries.

Run 1: *EPA Baseline - Random*

This run of 1,000 realizations establishes the EPA Baseline with fully random parameters. There are 520 WPs that have random early failure times between 1 and 5,000 years. The mean annual dose rises to 15 mrem/yr at 10,000 years. As in all Early Failure mode runs, the drip shields are not functional and I-129 and Tc-99 are included in the inventory. RunNumber is set to 0 for this run, permitting all parameters to vary. The output from this run is used for uncertainty and sensitivity analysis when all model parameters are permitted to vary according to their assigned probability distributions.

Run 2: *EPA Baseline-Medium Infiltration-Fixed*

This run establishes the EPA Baseline with all parameters fixed at their mean value. The deterministic medium infiltration case is selected. There are 520 WPs with a fixed early failure time at 2,500 years. The annual dose rises to 4.8 mrem/yr at 10,000 years. As in all other Early Failure mode runs, the drip shields are not functional. I-129 and Tc-99 are included in the inventory. For the fixed parameter runs, 10 realizations are generated to ensure that the model outputs are fixed, not random. RunNumber is set to 1 for this run, fixing all parameters at their mean value.

Run 3: *EPA Baseline-High Infiltration-Fixed*

This run is the same as Run 2, except the deterministic high infiltration case is selected.

Run 4: *EPA Baseline-Low Infiltration-Fixed*

This run is the same as Run 2, except the deterministic low infiltration case is selected.

Run 5: *Vary Seepage*

This run is the same as Run 2, except for the seepage parameters, which are permitted to vary across the full range of their assigned distributions. All other parameters are fixed at their mean value, including the early failure time, which is fixed at 2,500 years. The deterministic medium infiltration case is selected. The output from this run is used for uncertainty and sensitivity analysis when only seepage parameters are permitted to vary.

Run 6: *Vary Solubility*

This run is the same as Run 2, except the solubility parameters are permitted to vary across the full range of their assigned distributions. All other parameters are fixed at their mean value, including the early failure time at 2,500 years. The deterministic medium infiltration case is selected. The output from this run is used for uncertainty and sensitivity analysis when only solubility parameters are permitted to vary.

Run 7: *Vary Solubility & Seepage*

This run is the same as Run 2, except the seepage and solubility parameters are permitted to vary across the full range of their assigned distributions. All other parameters are fixed at their mean value, including the early failure time at 2,500 years. The deterministic medium infiltration case is selected. The output from this run is used only in Figure 15.

Run 8: *Vary Sol & Seep & Infiltration*

This run is the same as Run 2, except the seepage, solubility and infiltration parameters are permitted to vary across the full range of their assigned distributions. All other parameters are fixed at their mean value, including the early failure time at 2,500 years. The deterministic infiltration check box is not checked, so the infiltration case is selected randomly. The output from this run is used for uncertainty and sensitivity analysis when only seepage, solubility, and infiltration parameters are permitted to vary collectively.

Run 9: *Non-collapsed Drifts*

This sensitivity run is a fixed-parameter run identical to Run 2, except that the Non-collapsed drifts check box is checked. In all other runs, the drifts are assumed to collapse resulting in increased water flux through the wastes.

Run 10: *Baseline-No Early Failures*

This run has no early failures. Failures occur only by the general corrosion mechanism. All 11,384 waste packages are modeled.

Run 11: *QA-VT4 Random Nxxxx*

Run 11 comprises of a series of eight runs with increasing number of realizations, where the sample size is xxxx=300, 500, 1500, 2000, 2500, 3000, 4000, and 5000. Except for the sample size, all runs have model settings identical to those for Run 1, including the same initial seed. This series of runs, and Run 1 with n=1000, are used in Table 1 and Figures 5 and 6.

Run 12: *SZ Length 0*

In this sensitivity run, the length of the SZ is set to 0 using the check box on *Dashboard1*. The infiltration case is randomly selected. The results are used in Figure 8.

Run 13: *SZ Length 0 & High Infil*

This sensitivity run is the similar to Run 12, except the length of the SZ is set to 0 and the High deterministic infiltration case is selected. The results are used in Figure 8.

Run 14: *DOE Peak Dose Model-Nominal*

This run is the original DOE Peak Dose Model, with a few minor errors in the WP general corrosion model fixed. There are no early failures, only failures after 400,000 years due to general corrosion effects. All parameters vary randomly. This model does not include I-129 and Tc-99 in the inventory, and has no early failure mode. It uses 5,000-year time steps.

Run 15: *QA-VT5 Random with Fixed Eftime*

This run is the same as Run 1, except the time of early failures is fixed at 2,500 years rather than varying uniformly from 1 to 5,000 years.

Run 16: *QA-VT5 Fixed with Random Eftime*

This run is the same as Run 2, except the time of early failures is not fixed at 2,500 years but allowed to vary uniformly from 1 to 5,000 years.

Run 17: *QA-DOE Peak Dose Model-Nominal (4k time steps)*

This run of the DOE Peak Dose Model is the same as Run 14, except the time steps are changed to 4,000 years to match the EPA Uncertainty Model for calibration purposes.

Run 18: *EPA Baseline-Low Infiltration-Random*

This run is the same as Run 1, except the deterministic low infiltration case is selected rather than random infiltration. Results from this run are presented in Section 4.1 of the main report.

Run 19: *EPA Baseline-Med Infiltration-Random*

This run is the same as Run 1, except the deterministic medium infiltration case is selected rather than random infiltration. Results from this run are presented in Section 4.1 of the main report.

Run 20: *EPA Baseline-High Infiltration-Random*

This run is the same as Run 1, except the deterministic high infiltration case is selected rather than random infiltration. Results from this run are presented in Section 4.1 of the main report.

Run 21: *EPA Baseline-Random No LHS*

This run is the same as Run 1 except that the GoldSim Latin Hypercube Sampling (LHS) option, which is used in any run listed above with stochastic parameters, is turned off.

Table B-1. Conditions, Assumptions, and Check Box Selections for GoldSim Model Runs Included on Disks

Run ID / Run Name	# realizations	EF ⁽¹⁾ mode operational?	# WPs with early failure	Time of early failures (yr)	DS has no function?	Deterministic infiltration?	Infiltration case	Vary ⁽²⁾ seepage parameters?	Vary ⁽²⁾ solubility parameters?	Vary ⁽²⁾ other parameters?	I129 & Tc99 in inventory?	Non- collapsed drifts	SZ length of 0	Run ⁽³⁾ Number
1 EPA Baseline – Random ⁽⁴⁾	1000	√	520	0-5000	√	√	-	Y	Y	Y	Y	-	-	0
2 EPA Baseline – Medium Infiltration-Fixed ⁽⁵⁾	10	√	520	2500	√	√	Med √	N	N	N	Y	-	-	1
3 EPA Baseline – High Infiltration-Fixed	10	√	520	2500	√	√	High √	N	N	N	Y	-	-	1
4 EPA Baseline – Low Infiltration-Fixed	10	√	520	2500	√	√	Low √	N	N	N	Y	-	-	1
5 Vary Seepage	1000	√	520	2500	√	√	Med √	Y	N	N	Y	-	-	1
6 Vary Solubility	1000	√	520	2500	√	√	Med √	N	Y	N	Y	-	-	1
7 Vary Solubility & Seepage	1000	√	520	2500	√	√	Med √	Y	Y	N	Y	-	-	1
8 Vary Sol & Seep & Infiltration	1000	√	520	2500	√	√	-	Y	Y	N	Y	-	-	1
9 Non-collapsed Drifts	10	√	520	2500	√	√	Med √	N	N	N	Y	√	-	1
10 Baseline-no Early Failures	1000	-	0	n/a	-	-	-	Y	Y	Y	Y	-	-	0
11 QA-VT4 Random Nxxxx	300 to 5000	√	520	0-5000	√	-	-	Y	Y	Y	Y	-	-	0
12 SZ Length 0	1000	√	520	0-5000	√	-	-	Y	Y	Y	Y	-	√	0
13 SZ Length 0 & High Infil	1000	√	520	0-5000	√	√	High √	Y	Y	Y	Y	-	√	0
14 DOE Peak Dose Model-Nominal	1000	n/a	0	-	-	-	-	Y	Y	Y	N	-	-	n/a
15 QA-VT5 Random with fixed Eftime	1000	√	520	2500	√	-	-	Y	Y	Y	Y	-	-	0
16 QA-VT5 Fixed with random Eftime	10	√	520	0-5000	√	√	Med √	N	N	N	Y	-	-	1

Table B-1. Conditions, Assumptions, and Check Box Selections for GoldSim Model Runs Included on Disks

Run ID / Run Name	# realizations	EF ⁽¹⁾ mode operational?	# WPs with early failure	Time of early failures (yr)	DS has no function?	Deterministic infiltration?	Infiltration case	Vary ⁽²⁾ seepage parameters?	Vary ⁽²⁾ solubility parameters?	Vary ⁽²⁾ other parameters?	1129 & Tc99 in inventory?	Non- collapsed drifts	SZ length of 0	Run ⁽³⁾ Number
17 QA-DOE Peak Dose Model (4k time steps)	1000	n/a	0	n/a	-	-	-	Y	Y	Y	N	-	-	n/a
18 EPA Baseline-Low Infiltration-Random	1000	√	520	0-5000	√	√	Low √	Y	Y	Y	Y	-	-	0
19 EPA Baseline-Med Infiltration-Random	1000	√	520	0-5000	√	√	Med √	Y	Y	Y	Y	-	-	0
20 EPA Baseline-High Infiltration-Random	1000	√	520	0-5000	√	√	High √	Y	Y	Y	Y	-	-	0
21EPA Baseline-Random no LHS	1000	√	520	0-5000	√	-	-	Y	Y	Y	Y	-	-	0

¹ Checkbox controls are set on Dashboard1 of the GoldSim model. The GoldSim model name for each model run on the disk is: Run Name (version/notes).gsm. Each model is accompanied by its corresponding version of the Excel workbook named SelectValue.xls.

² Parameter variation is enabled by entering a Forced RunNumber of 0 in the appropriate rows of the Summary worksheet of the specific version of SelectValue.xls included in the subdirectory with each GoldSim model.

³ When the RunNumber parameter is 1, all stochastic parameters are fixed to their mean value, except for the parameters with Forced RunNumbers specified on the Summary worksheet of the SelectValue.xls workbook. When the RunNumber parameter is 0, all parameters are permitted to vary over their assigned distributions. (Also see footnote 5.)

⁴ The EPA Baseline model with all random parameters has a mean annual dose of approximately 15 mrem/yr at 10,000 years.

⁵ When parameters are “fixed,” (i.e., RunNumber=1) all continuous stochastic parameters are set to their mean values found in SelectValue.xls; Starting_Water_Chemistry is set to ‘3’ (CS1000); Cracks_Before_Patches is set to ‘TRUE’; and Barrier Failure Type = ‘Predicted Failure Time’ is selected on the Contaminant Transport tab of the GoldSim main menu Model | Options window. When RunNumber=0, all parameters are random.

Table B-2. Directory Location and Use in Report of GoldSim Model Runs Included on Disks

Run ID / Run Name	Directory location on Disk	Use in Report
1 EPA Baseline - Random	\EPA Baseline\Random Parameters\	Figures 2,4,7,21,22;23; Tables 10,13,14
2 EPA Baseline-Medium Infiltration-Fixed	\EPA Baseline\Fixed Parameters\Medium Infiltration\	Figure 9; Table 3
3 EPA Baseline-High Infiltration-Fixed	\EPA Baseline\Fixed Parameters\High Infiltration\	Table 3
4 EPA Baseline-Low Infiltration-Fixed	\EPA Baseline\Fixed Parameters\Low Infiltration\	Table 3
5 Vary Seepage	\Sensitivity Runs\Vary Seepage Parameters\	Figures 10,12,16,17,18, 19; Tables 4,5,10
6 Vary Solubility	\Sensitivity Runs\Vary Solubility Parameters\	Figures 13,14,16,17,18, 19; Tables 7,8,9,10
7 Vary Solubility & Seepage	\Sensitivity Runs\Vary Solubility & Seepage\	Figure 15
8 Vary Sol & Seep & Infiltration	\Sensitivity Runs\Vary Solubility & Seepage & Infiltration\	Figures 16,17,18,19, 20; Tables 10,11,12
9 Non-collapsed Drifts	\Sensitivity Runs\Non-collapsed Drifts\	Figure 11
10 EPA Baseline-no Early Failures	\QA\Calibration Runs\	Figure 3
11 QA-VT4 Random N _{xxxx} ¹	\QA\Validation Tests\Test 4	Table 1; Figures 5,6
12 SZ Length 0	\Sensitivity Runs\SZ Length Zero\	Figure 8
13 SZ Length 0 & High Infil	\Sensitivity Runs\SZ Length Zero & High Infiltration\	Figure 8
14 DOE Peak Dose Model-Nominal	\DOE Peak Dose Model\	Figure 1
15 QA-VT5-Random with fixed Eftime	\QA\Validation Tests\Test 5	Table 2
16 QA-VT5 Fixed with random Eftime	\QA\Validation Tests\Test 5	Table 2
17 QA-DOE Peak Dose Model (4K yr steps)	\QA\Validation Tests\Test 3	Figure 3
18 EPA Baseline-Low Infiltration-Random	\EPA Baseline\Random Parameters\Low Infiltration\	Section 4.1
19 EPA Baseline-Med Infiltration-Random	\EPA Baseline\Random Parameters\Medium Infiltration\	Section 4.1
20 EPA Baseline-High Infiltration-Random	\EPA Baseline\Random Parameters\High Infiltration\	Section 4.1
21 EPA Baseline-Random no LHS ²	\QA\Validation Tests\Test 6	Table 2

¹ Series of eight runs starting from the same seed, where xxx=300, 500, 1500, 2000, 2,500, 3000, 4000, or 5000 realizations.

² GoldSim Latin Hypercube Sampling (LHS) option is selected in all other runs with stochastic parameters for efficient estimation of the mean annual dose. LHS is not selected in Run 21.

Table B-3. Parameters in All-Parameter Regression not Included in Other Stepwise Regressions

ID	Parameter Name	GoldSim Module
1	Ac227_BDCF	\Biosphere
2	Alluvium_Density	\Saturated_Zone
3	CORAL	\Saturated_Zone
4	Cracks_Before_Patches	\Source_Term_Models
5	CSNF_Inventory_Unct	\Source_Term_Models
6	CSNF_pH_Greater_600	\Source_Term_Models
7	CSNF_pH_Less_600	\Source_Term_Models
8	DCVO	\Saturated_Zone
9	DSNF_Inventory_Unct	\Source_Term_Models
10	Early_Failure_Time	\EF_and_Test_Functions
11	FISVO	\Saturated_Zone
12	Flux_Split_Uncertainty	\Source_Term_Models
13	FPLAW	\Saturated_Zone
14	GWSPD	\Saturated_Zone
15	HAVO	\Saturated_Zone
16	HLW_Inventory_Unct	\Source_Term_Models
17	I129_BDCF	\Biosphere
18	Kd_I_FeOx_CP	\Source_Term_Models
19	Kd_Np_Al	\Saturated_Zone
20	Kd_Np_FeOx_CP	\Source_Term_Models
21	Kd_Np_Invert	\Source_Term_Models
22	Kd_Pa_FeOx_CP	\Source_Term_Models
23	Kd_Pa_Invert	\Source_Term_Models
24	Kd_Pu_Al	\Saturated_Zone
25	Kd_Pu_FeOx_CP	\Source_Term_Models
26	Kd_Pu_Invert	\Source_Term_Models
27	Kd_Ra_Al	\Saturated_Zone
28	Kd_Tc_FeOx_CP	\Source_Term_Models
29	Kd_Th_Al	\Saturated_Zone
30	Kd_Th_FeOx_CP	\Source_Term_Models
31	Kd_Th_Invert	\Source_Term_Models
32	Kd_U_Al	\Saturated_Zone

Table B-3. Parameters in All-Parameter Regression not Included in Other Stepwise Regressions

ID	Parameter Name	GoldSim Module
33	Kd U FeOx CP	\Source Term Models
34	Kd U Invert	\Source Term Models
35	LDISP	\Saturated Zone
36	MIC Factor	\WPandDS Degradation Model
37	Np237_BDCF	\Biosphere
38	NVF19	\Saturated Zone
39	Pa231_BDCF	\Biosphere
40	pH_CDSP_High_Q	\Source Term Models
41	pH_CDSP_Low_Q	\Source Term Models
42	Pu239_BDCF	\Biosphere
43	Pu240_BDCF	\Biosphere
44	Pu242_BDCF	\Biosphere
45	Ra226_BDCF	\Biosphere
46	Schoepite_Porosity	\Source Term Models
47	Starting_Water_Chemistry	\Source Term Models
48	Tc99_BDCF	\Biosphere
49	Th229_BDCF	\Biosphere
50	Th230_BDCF	\Biosphere
51	Th232_BDCF	\Biosphere
52	U233_BDCF	\Biosphere
53	U234_BDCF	\Biosphere
54	U236_BDCF	\Biosphere
55	U238_BDCF	\Biosphere

Table B-4. Parameters Not Selected by All-Parameter Stepwise Regression

ID	Parameter Name	Coefficient	t Statistic	Significance Level
1	Ac227 BDCF	0.019	1.312	0.190
2	Alluvium_Density	-0.004	-0.293	0.769
3	CORAL	-0.011	-0.765	0.445
4	Cracks_Before_Patches	0.022	1.566	0.118
5	CSNF_Inventory_Unct	0.006	0.444	0.657
6	CSNF_pH_Greater_600	0.003	0.183	0.855
7	CSNF_pH_Less_600	-0.019	-1.306	0.192
8	DCVO	-0.007	-0.459	0.647
9	DSNF_Inventory_Unct	0.011	0.764	0.445
10	Early_Failure_Time	0.008	0.587	0.558
11	FISVO	-0.006	-0.406	0.685
12	Flux_Split_Uncertainty	-0.017	-1.174	0.241
13	I129_BDCF	0.005	0.347	0.729
14	Kd_I_Invert	-0.016	-1.102	0.271
15	Kd_Np_Al	0.014	0.973	0.331
16	Kd_Np_FeOx_CP	-0.012	-0.804	0.421
17	Kd_Np_Invert	0.004	0.296	0.767
18	Kd_Pa_FeOx_CP	0.014	0.990	0.323
19	Kd_Pa_Invert	0.012	0.843	0.399
20	Kd_Pu_Invert	-0.018	-1.219	0.223
21	Kd_Ra_Al	0.012	0.872	0.384
22	Kd_Tc_Invert	0.008	0.565	0.572
23	Kd_Th_Al	-0.007	-0.465	0.642
24	Kd_Th_FeOx_CP	-0.009	-0.634	0.526
25	Kd_U_Al	-0.006	-0.407	0.684
26	Kd_U_FeOx_CP	0.017	1.208	0.227
27	Kd_U_Invert	0.001	0.055	0.956
28	LDISP	-0.002	-0.158	0.874
29	Log_Np_Sol_eps2_NpO2_CDSP_I	-0.023	-1.600	0.110
30	Log_Np_Sol_eps2_NpO2_CSNF	-0.010	-0.708	0.479
31	Log_Pa_Sol_eps1	-0.021	-1.444	0.149

Table B-4. Parameters Not Selected by All-Parameter Stepwise Regression

ID	Parameter Name	Coefficient	t Statistic	Significance Level
32	Log_Pa_Sol_eps2_CDSP	0.003	0.234	0.815
33	Log_Pa_Sol_eps2_CSNF	-0.017	-1.184	0.237
34	Log_Pu_Sol_eps2_CDSP	-0.006	-0.389	0.697
35	Log_Pu_Sol_eps2_CSNF	-0.002	-0.169	0.866
36	Log_Th_Sol_eps1	0.006	0.443	0.658
37	Log_Th_Sol_eps2_CDSP	0.004	0.306	0.760
38	Log_Th_Sol_eps2_CSNF	0.010	0.705	0.481
39	Log_U_Sol_eps1	0.005	0.314	0.754
40	Log_U_Sol_eps2_CDSP_S	0.028	1.934	0.053
41	Log_U_Sol_eps2_CSNF	0.013	0.933	0.351
42	MIC_Factor	0.020	1.402	0.161
43	Pa231_BDCF	0.016	1.087	0.277
44	pH_CDSP_Low_Q	-0.005	-0.351	0.726
45	Pu240_BDCF	0.002	0.121	0.904
46	Ra226_BDCF	0.008	0.586	0.558
47	Schoepite_Porosity	-0.003	-0.237	0.813
48	Starting_Water_Chemistry	0.007	0.486	0.627
49	Th229_BDCF	0.015	1.019	0.308
50	Th232_BDCF	0.015	1.046	0.296
51	U_Sol_Pick	0.001	0.043	0.966
52	U234_BDCF	0.027	1.865	0.062
53	U236_BDCF	0.010	0.710	0.478
54	U238_BDCF	0.009	0.649	0.517