SUPPLEMENTAL PERFORMANCE ANALYSES FOR THE POTENTIAL HIGH-LEVEL NUCLEAR WASTE REPOSITORY AT YUCCA MOUNTAIN

S. David Sevougian, Jerry A. McNeish
Duke Engineering & Services, Inc.
1180 Town Center Drive, Las Vegas, NV 89144

Kevin Coppersmith
Coppersmith Consulting, Inc.
2121 N. California Blvd., #290, Walnut Creek, CA 94596

Karen E. Jenni
Geomatrix Consultants, Inc.
2101 Webster Street, 12th floor, Oakland, CA 94612

Larry D. Rickertsen
Bechtel-SAIC Company, LLC.
1180 Town Center Drive, Las Vegas, NV 89144

Peter N. Swift, Michael L. Wilson
Sandia National Laboratories
P.O. Box 5800, Albuquerque, NM, 87185-0778

ABSTRACT

The U.S. Department of Energy (DOE) is considering the possible recommendation of a site at Yucca Mountain, Nevada, for the potential development of a geologic repository for the disposal of high-level radioactive waste and spent nuclear fuel. To facilitate public review and comment, in May 2001 the DOE released the *Yucca Mountain Science and Engineering Report* (S&ER) (1), which presents technical information supporting the consideration of the possible site recommendation. The report summarizes the results of more than 20 years of scientific and engineering studies.

Based on internal reviews of the S&ER and its key supporting references, the *Total System Performance Assessment for the Site Recommendation* (TSPA-SR) (2) and the Analysis Model Reports and Process Model Reports cited therein, the DOE has recently identified and performed several types of analyses to supplement the treatment of uncertainty in support of the consideration of a possible site recommendation. The results of these new analyses are summarized in the two-volume report entitled *FY01 Supplemental Science and Performance Analysis* (SSPA) (3,4). The information in this report is intended to supplement, not supplant, the information contained in the S&ER. The DOE recognizes that important uncertainties will always remain in any assessment of the performance of a potential repository over thousands of years (1). One part of the DOE approach to recognizing and managing these uncertainties is a commitment to continued testing and analysis and to the continued evaluation of the technical basis supporting the possible recommendation of the site, such as the analysis contained in the SSPA.

The goals of the work described here are to provide insights into the implications of newly quantified uncertainties, updated science, and evaluations of lower operating temperatures on the performance of a potential Yucca Mountain repository and to increase confidence in the results of the TSPA described in the S&ER (1). The primary tool used to evaluate the implications of the three types of supplemental information described in the SSPA (3,4) is the Yucca Mountain integrated TSPA model.

In the SSPA two types of analyses of the performance of the potential repository were conducted using the TSPA model. First, a set of "one-off" sensitivity analyses was conducted to evaluate the effects of incorporating the updated models and representations one at a time. Then, the updated models and representations were abstracted and aggregated to produce a modified TSPA model, referred to as the supplemental TSPA model, which captures the combined effects of those alternative representations. This supplemental TSPA model was used to evaluate system performance over a range of thermal operating modes. The supplemental TSPA model results were compared with results of the TSPA-SR to provide insights into the cumulative effects of all model changes on the system results and to demonstrate that the TSPA-SR analyses were conservative in nature, i.e., that a safety margin had been built into the suite of TSPA-SR models.

INTRODUCTION

Performance assessment is a method of forecasting how a potential repository system, designed to contain radioactive waste, is expected to behave over time. One goal of performance assessment is to aid in determining whether the potential repository system can meet established performance requirements. Other applications include identifying which barriers and processes significantly affect performance, explicitly presenting uncertainty in projections, and providing information to guide future design and testing activities. The TSPA is a comprehensive quantitative analysis where the results of detailed conceptual and numerical models of each of the individual and coupled processes are combined into a single probabilistic model that can be used to project how a potential repository will perform over time. Detailed background on the definition, philosophy, regulatory requirements for, and the development and use of a TSPA is described in the *Total System Performance Assessment for the Site Recommendation* (TSPA-SR) (2).

Because it is not possible to have perfect knowledge or understanding of all the components of the disposal system, and because of the long time scales of interest, estimates of repository performance can never be certain. Thus, in considering the safety of a potential disposal site for high-level waste, it is important to take into account the effect of uncertainties on the conclusions.

The primary tool being used for uncertainty analysis of potential Yucca Mountain repository performance is the Monte Carlo method. The uncertainties of key model input parameters are quantified by assigning probability distributions to them. The total-system model is then run for multiple realizations of the system. Each realization represents a possible future history of the disposal system and has a unique set of values for the uncertain parameters, sampled from their distributions. Monte Carlo simulations are computed separately for the nominal, igneous-disruption, and human-intrusion scenario classes (2). Results for the nominal and disruptive scenario classes can be combined (with appropriate probability weighting) to obtain the overall mean annual dose, which is the quantity to be compared with U.S. regulatory standards (5). Although the mean of the dose distributions is the key quantity specified by regulation, the entire distribution is of interest, because the distribution represents a quantification of the uncertainty in projected dose. Realizations that produce high dose estimates are of particular interest, and can be examined to determine the particular combinations of input values that lead to high calculated doses. In addition, results for each simulation can be examined in detail, including analysis of correlations of input parameters with the computed annual dose at various times, in order to determine which parameters and models have the greatest influence on the results.

TSPA results can be reviewed at the system level and at the subsystem level. System-level results refer to one of the key outputs of the TSPA model: estimated annual dose from radiological exposure to materials released from the potential repository and received by a critical group of individuals that reside on a transport pathway from the potential repository to the biosphere. System-level TSPA analyses produce estimates of the annual dose over the time of the analyses. Subsystem-level results refer to intermediate results of the TSPA model. Intermediate results include, for example, the seepage rate of liquid through the emplacement drift wall or the transport time of specific radionuclides in the saturated zone. Subsystem- and system-level results can provide insight into the effect of newly-quantified uncertainties, newly-updated technical and scientific information, and potential impacts of changes in thermal operating mode. Both total system and subsystem analyses are included in the TSPA-SR and the SSPA.

Sensitivity analyses make it possible to trace a specific model update to a specific change in system-level results, i.e., to a change in estimated expected annual dose. Because the results produced at the system level are dose estimates, these system-level sensitivity analyses can result in insights about the overall degree of conservatism or non-conservatism in the results of other analyses using TSPA models. In cases where sensitivity analyses do not show impacts on the system-level results, analyses that are focused on subsystem-level results help to isolate and show the immediate implications of model updates. The subsystem-level analyses emphasize the impact on intermediate results where changes can be tied most directly to the specific process model updates being evaluated. However, subsystem-level results can also provide insights into the importance of the specific input to system-level performance, and into the degree of conservatism or non-conservatism in previous model assumptions. For example, if an updated representation involves making a large change to an input parameter to a process (i.e., subsystem) model, and the results of that process model or the abstracted model change little or not at all, then system performance will not be sensitive to that particular input. Thus, subsystem results can be used to provide insights into whether the updated representations have the potential to impact the overall total system performance. These conclusions need to be made cautiously. Many of these sensitivity analyses were run individually, and individually many showed little effect, but it is possible that combinations of parameters might have a larger effect.

METHODS AND APPROACH

In general, the studies and analyses described in this document provide additional information of three types:

- **Unquantified Uncertainties Analysis**–Specific uncertainties that were not treated explicitly in the S&ER and the TSPA-SR are quantified. Unquantified uncertainties include parameter bounds, conceptual models, assumptions, and in some cases, input parameters consisting of statistically biased or skewed distributions. The primary goals of this effort were to provide insights into the importance of the unquantified uncertainties and the degree of conservatism in the overall assessment of the performance of a potential repository in the TSPA-SR.

- **Updates in Scientific Information**–New information has been developed for some of the process models that are important to repository performance. This work includes new experimental results, new conceptual models, and new analytical approaches, as well as results of continued research. It also includes identification and discussion of multiple lines of evidence that have been used directly, to support modeling, or indirectly, to develop confidence in modeling results. The primary goals of this effort were to provide insights into the impact of the new scientific results and improved models (i.e., those updated since completion of the models supporting the S&ER), and to develop additional confidence in the models and parameters used for total system performance assessment.

- **Lower-Temperature Operating Mode [LTOM] Analysis**–Because some of the processes that can affect performance are a function of the environment in the potential repository (e.g., temperature and humidity), the uncertainties associated with models of these processes also depend on the environmental variables. In particular, operating the potential repository at temperatures above 96°C would result in water boiling and condensing, which requires models

> of flow and transport that are more complex—and possibly more uncertain—than models at lower temperatures. Therefore, the effects of a range of thermal operating modes on projected system performance, including lower operating temperatures in the potential repository (e.g., below 96°C at the drift wall or below 85°C at the waste package surface), have been evaluated. The uncertainties associated with various process models have been analyzed over a range of temperatures. The primary goals of evaluating a range of thermal operating modes were to provide insights into the effect of thermal parameters on predicted performance of a potential repository, including uncertainty of those predictions, and to increase confidence in the predicted performance of a potential repository over a range of thermal conditions.

In the supplemental performance evaluations (4), the updated conceptual and process models described in SSPA Volume 1 (3) were abstracted and incorporated into a TSPA model using a process identical to the abstraction process described in detail in the TSPA-SR (2). Two types of analyses were conducted: (1) *TSPA sensitivity analyses,* which refer to TSPA analyses wherein only one or a few components of the TSPA-SR model are updated with the newly abstracted models and the subsequent results compared with the TSPA-SR results; and (2) many or most of the updated component models are combined with the original TSPA-SR model to produce the *SSPA supplemental TSPA model*, whose results (both total system and subsystem) are compared to the TSPA-SR model. The methods and approach for both types of analyses are described below.

TSPA Sensitivity Analyses

TSPA sensitivity analyses were conducted for some of the updated models or representations described in SSPA Volume 1 (3, Table 1.3-1). TSPA sensitivity analyses were conducted for those updated models or representations judged by the Yucca Mountain Project Site Characterization Project (YMP) to have the potential to influence TSPA results based on analyses described in SSPA Volume 1. For each of the topics indicated for TSPA sensitivity analysis, the updated representations were abstracted and incorporated into the TSPA-SR model one at a time. One-off sensitivity analyses were conducted to evaluate the implications of each of the model changes on the estimated performance (dose) of the potential repository. All of the one-off sensitivity analyses used the TSPA-SR nominal scenario (i.e., the expected repository behavior through time in the absence of unlikely disruptive events such as volcanism) as the basis for comparison.

Sensitivity analyses make it possible to trace a specific model update to a specific change in system-level results, that is, to a change in estimated expected annual dose. Because the results produced at the system level are dose estimates, these system-level sensitivity analyses can result in insights about the overall degree of conservatism or non-conservatism in other TSPA model results. Sensitivity analyses focused on subsystem-level results help to isolate and show the implications of model updates. They emphasize the impact on intermediate results where changes can be tied most directly to the specific process model updates being evaluated.

SSPA Supplemental TSPA Model

Comparing the results of the TSPA sensitivity analyses with the results of the TSPA-SR model illustrates the impact of the supplemental information for individual topics in isolation. To gain insights into cumulative and coupled effects when several of the model components are updated, the SSPA supplemental TSPA model was developed. Of the many component models that were updated due to quantification of uncertainties, updated science, or revised thermal conditions, only some of the changes were incorporated into the SSPA supplemental TSPA model. In deciding which topics to include in this SSPA supplemental TSPA model, the YMP used the results of TSPA sensitivity analyses and professional judgement and experience with TSPA models to select those topics which had the greatest potential impact on performance (expected annual dose history), those judged to be the most sensitive to thermal effects, and those which were deemed most important by external reviewers. Results of the SSPA supplemental TSPA model are compared with results of the TSPA-SR. These comparisons provide insights into the cumulative effects of multiple model changes on system results and add to the insights on the implications of the supplemental information resulting from the TSPA one-off sensitivity analyses.

The SSPA supplemental TSPA model also provides the platform for a set of thermal sensitivity analyses. The goals for developing and evaluating the supplemental information on the LTOM were to provide insights into the effect of thermal parameters on predicted performance of the potential repository, including uncertainty in those predictions, and to increase confidence in the predicted performance of the potential repository over a range of thermal conditions. The design and mode of operations for the potential repository described in the S&ER are expected to be flexible enough to meet a range of potential thermal conditions or goals. For process models where thermal load potentially has an impact on the modeling and model results, analyses were conducted to evaluate the manner in which the process models, parameters, and results would vary under different thermal loading, focusing particularly on an LTOM. Two thermal operating modes were evaluated with the SSPA supplemental TSPA model: (1) the thermal operating mode described in the S&ER (the higher-temperature operating mode [HTOM]); and (2) an alternative LTOM wherein average maximum temperatures on the waste package do not exceed 85ºC following closure of the potential repository. The expected annual dose estimates from these two SSPA supplemental TSPA model implementation are compared directly to gain insight into differences in performance that may result from different thermal operating conditions.

Finally, the subsystem-level analyses conducted with the supplemental TSPA model include examinations of the subsystem performance to changes due to thermal operating modes. These show which components of the total system are sensitive to temperatures in the potential repository, and show the implications of different thermal modes for performance at the subsystem level. This can be important in that some processes may be thermally affected but that effect may only be discernable at the subsystem level and not at the system level. Again, conclusions about the system-level implications of different thermal operating modes based on subsystem-level results must be made cautiously. Since many of these sensitivity analyses are being run individually, there is a possibility that coupled processes will not be captured in these subsystem-level analyses.

TSPA SENSITIVITY ANALYSES: EVALUATIONS OF UNCERTAINTY AND NEW INFORMATION

This section describe results of three one-off sensitivity analyses conducted by modifying the models and input parameters used in the TSPA-SR base-case (2). Except for the model or parameter being examined, these one-off sensitivity analyses were conducted using the same models and input parameters as those used in TSPA-SR base-case, and therefore differences in performance measures between these results and those of the TSPA-SR provide insights into the importance of uncertainty in individual model components. The results are displayed here as system-level annual dose histories for nominal performance. All analyses described in this section use 100 realizations of the TSPA model.

As mentioned above, the TSPA-SR nominal scenario is the basis of comparison for the one-off sensitivity studies. Results of the TSPA-SR for nominal performance have been documented in detail (2). The nominal performance scenario includes all features, events, and processes that are expected to occur during the first 10,000 years, but it does not include human intrusion or unlikely disruptive events. The TSPA-SR nominal performance analyses address two periods: (1) 100,000 years after waste emplacement; and (2) 1,000,000 years after waste emplacement. The first period focuses on performance for 10,000 years, with the analyses extended to 100,000 years to evaluate robustness of the system with respect to 10,000-year performance. The second period is considered to evaluate the peak annual dose, which occurs between 100,000 and 1,000,000 years in most realizations.

The TSPA-SR base-case model was developed to provide a defensible basis for evaluating 10,000-year performance, rather than to provide a realistic evaluation of uncertainty in peak dose. The TSPA-SR therefore included sensitivity analyses of 1,000,000-year performance to examine the effects of more realistic alternative models for long-term climate change and secondary-phase effects on actinide solubilities (2). These sensitivity analyses have been superseded by the results of more recent analyses described here.

As mentioned earlier, there were three types of information included in the SSPA analyses: (1) quantification of previously unquantified uncertainties; (2) newly available scientific data; and (3) the addition of temperature dependencies to some of the models. All three types of information were not necessarily included in each and every supplemental model. In fact, of the three supplemental models discussed below, the first one (new solubility limits) is an example where all three types were included, while the second supplemental model (transport through the engineered barrier system [EBS]) is an example where only the first two types were included (newly quantified uncertainties and new science) and the third example (drift shadow zone) is an example of only newly quantified uncertainties.

In-Package Radionuclide Solubility Limits

The model for dissolved radionuclide concentration limits is described in the TSPA-SR (2). These solubility limits are calculated from the in-package chemical conditions, specification of the mineral phases that control the solubility of the elements under consideration, and the thermodynamic parameters that govern the stability of the aqueous species and mineral phases. Uncertainty taken into account in the estimate of the in-package chemistry is considered in developing the values for the solubility limits. For americium, neptunium, and uranium, the uncertainty in the chemistry is explicitly taken into account. For the others, bounding values are used for the in-package chemistry parameters. In addition, sensitivity to the selection of controlling phases is considered for neptunium and thorium.

The new supplemental solubility model considered here has a wider range for the uncertainty in the effect of the controlling phases for plutonium, neptunium, thorium, and technetium. The effects of the extended range of uncertainty in these concentration limits, along with the effects on in-package chemistry (e.g., pH), are shown in Fig. 1. Fig. 1a compares the mean annual dose taking these effects into account with the results using the base-case model. Fig. 1b shows the contributions of the various radionuclides to the total mean annual dose estimate when these effects are taken into account.

The results show significant changes after the waste packages are breached. As determined in the TSPA-SR (2) Neptunium-237 (^{237}Np) dominates the annual dose estimate in the nominal scenario; therefore, changes to the solubility limit of this radionuclide have a large effect on the estimate of total mean annual dose. The new model accounts for two compensating changes. The change in the neptunium solubility limit, independent of the change in chemistry, would lower the annual dose from this radionuclide. However, a reduction in pH of the water in the waste package tempers this reduction. As a result, the mean annual dose for ^{237}Np is reduced by more than an order of magnitude.

The estimates for other radionuclides also are reduced by the changes in solubility limits. In particular, the mean annual dose from the plutonium isotopes is reduced by about a factor of three. The overall effect of these changes is to reduce the estimate of total mean annual dose by a factor of more than five.

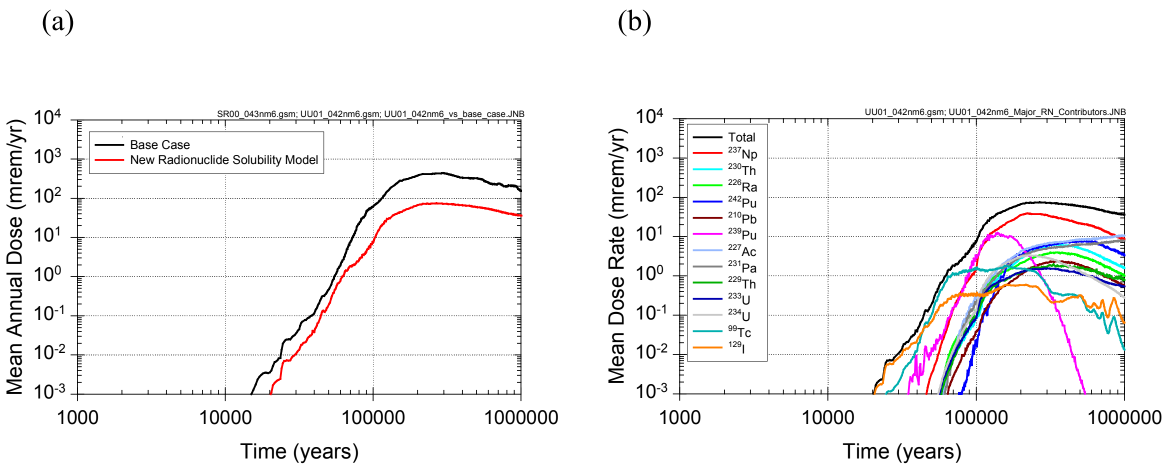

Fig. 1. Radionuclide solubility sensitivity case: (a) Comparison of mean annual dose between the SSPA radionuclide solubility model and the TSPA-SR base case model; and (b) Contribution of individual radionuclides to the mean annual dose for the SSPA radionuclide solubility model.

Analyses of Radionuclide Transport in the Engineered Barrier System (EBS)

The TSPA-SR base-case model for radionuclide transport in the EBS accounts for transport of dissolved and colloid-associated radionuclides and considers advective and diffusive transport of these concentrations radionuclides through the EBS. However, the TSPA-SR base-case model does not account for resistance to release due to transport processes within the waste package. A model for diffusive transport on thin films on the surface of in-package components is considered in the SSPA, along with an improved representation for the diffusivity of the drift invert (3,4). Results implementing these two effects are shown in Fig. 2a.

There is little difference between the dose calculated using the base-case model and the new model for diffusive transport in the EBS. One possible reason for the small difference in these two estimates is the diffusion coefficient used for transport within the waste package. The diffusion coefficient used in the analysis is conservative and sensitivity analyses on the value of the diffusion coefficient generally show this conservatism to be important. For example, sensitivity analyses in the TSPA-SR (2) for the diffusion coefficient of the drift invert show that diffusion plays a key role in the EBS transport even after the drip shield and waste package have breached. This conclusion is sensitive to the diffusion properties assumed for the invert. The TSPA-SR base-case model uses a conservative representation for the invert diffusivity, and the sensitivity analyses indicate diffusive mass transport exceeds advective mass transport at early times and is comparable to it in the long term. Analyses using a more realistic diffusivity have lower diffusive mass transport. As in the analysis of the invert diffusion properties, a conservatively high diffusion coefficient in the waste package results in limited diffusion resistance to radionuclide transport.

The second new model for EBS transport is the effect of sorption on radionuclide transport in the EBS, in particular, the effect of iron corrosion products on reversible and irreversible sorption in the invert. The TSPA-SR base-case model assumes no sorption of dissolved species within the EBS. However, the SSPA Volume 1 (3) discusses the conservative nature of this assumption and develops a model for the sorption of radionuclides in the EBS, including sorption partition coefficients (K_ds) for corrosion products and other materials within the waste package and drift invert and fractions of radionuclides irreversibly sorbed onto these materials. Results using these new K_ds are shown in Fig. 2b.

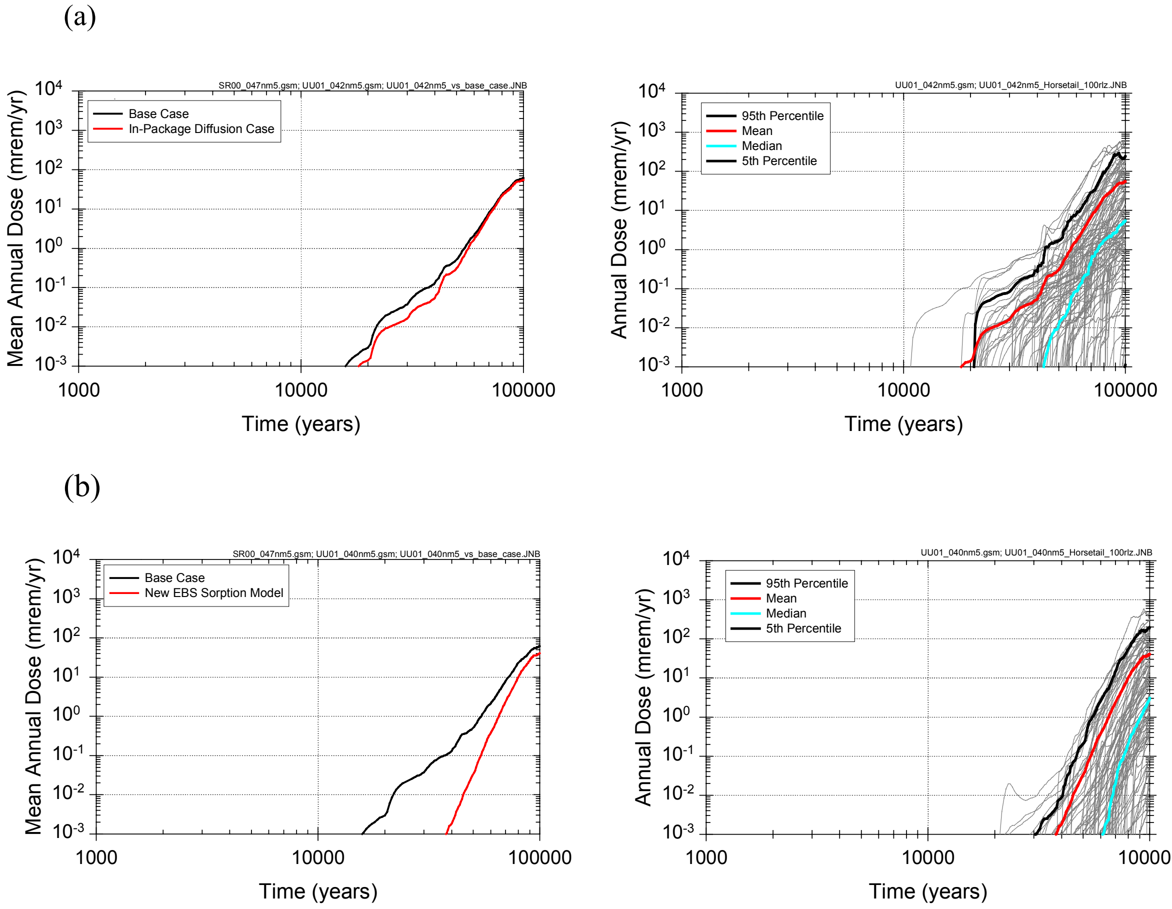

Fig. 2. EBS transport sensitivity case: (a) Comparison of mean annual dose between the SSPA in-package diffusion model and the TSPA-SR base case (left), and range of results for all 100 realizations of the mean annual dose history for the SSPA in-package diffusion model (right); and (b) Comparison of mean annual dose between the SSPA EBS sorption model and the TSPA-SR base case (left), and range of results for all 100 realizations of the mean annual dose history for the SSPA EBS sorption model (right).

The reduction in mean annual dose from the TSPA-SR base-case derives primarily from the reduction in concentrations in the liquid phase due to the partitioning of the concentrations between the liquid phase and the solid phases. This reduces both diffusive and advective mass transport away from the source—the former via a reduced concentration gradient between the waste form source and the host rock beneath the drift and the latter via a reduced aqueous concentration in the liquid flowing through the waste package

Evaluation of Unsaturated Zone Transport

Unsaturated zone (UZ) transport refers to the movement of radionuclides from the potential repository, through the UZ, and to the water table. UZ transport is the first natural barrier to radionuclides that escape from the potential repository. UZ transport acts as a barrier by delaying radionuclide movement. If the transport time is large compared to the half-life of a radionuclide, then the UZ can have a large effect on decreasing the dose from that radionuclide at the biosphere.

Within a TSPA simulation, UZ flow is modeled as a sequence of steady states (2); however, the transport calculation itself is fully transient. A dual-continuum conceptual model is used for transport, with fractures and rock matrix represented as two interacting continua. In the TSPA-SR base-case model, radionuclide releases from the EBS (invert) are released into the fracture continuum of the UZ transport model. This choice is conservative in that fracture transport is faster than matrix transport. However, the region directly beneath an emplacement drift is expected to be drier at ambient conditions than the host formation at this depth because of the diversion of water around the drift opening due to the drift capillary-barrier effect. Such perturbations of flow (primarily fracture flow) caused by the presence of the drifts are neglected in the UZ-transport component of the TSPA-SR model, since all radionuclides are released into the fractures of the host rock. Neglecting this flux “shadow” below the drift is thus conservative because the drier conditions at the interface between the EBS and the UZ would increase transport times if included.

As an initial estimate of the effect of the presence of the drift on UZ transport, a sensitivity analysis was performed in which only advective releases from the potential repository were released into the fracture continuum of the UZ transport model, as in the TSPA-SR base-case, but diffusive releases were released into the matrix continuum of the model instead (3). The rationale for placement of diffusing radionuclides into the matrix rather than the fractures is that the area for diffusion at the drift boundary is roughly proportional to the water content, and the matrix-water content is approximately 1,000 times greater than the fracture-water content (3). This approximation for including the drift shadow may be somewhat conservative because the ambient fracture and matrix flow fields are used for transport (i.e., the reduction in flow below the drifts is not taken into account). In contrast, another aspect of the method related to the implementation of matrix diffusion (radionuclides that have entered the matrix are not allowed to diffuse to the fractures) may be nonconservative (3).

The results of this sensitivity analysis are shown in a comparison of the mean annual dose for this case with that of the TSPA-SR base-case (Fig. 3). The results show a delay of approximately 10,000 years in the mean annual dose for the drift-shadow case as compared to the TSPA-SR base-case. The effect is as large as it is because a large portion of the radionuclide releases are diffusive, especially for Technicium-99 (^{99}Tc) (2), and because transport through the matrix is slower than transport through the fractures.

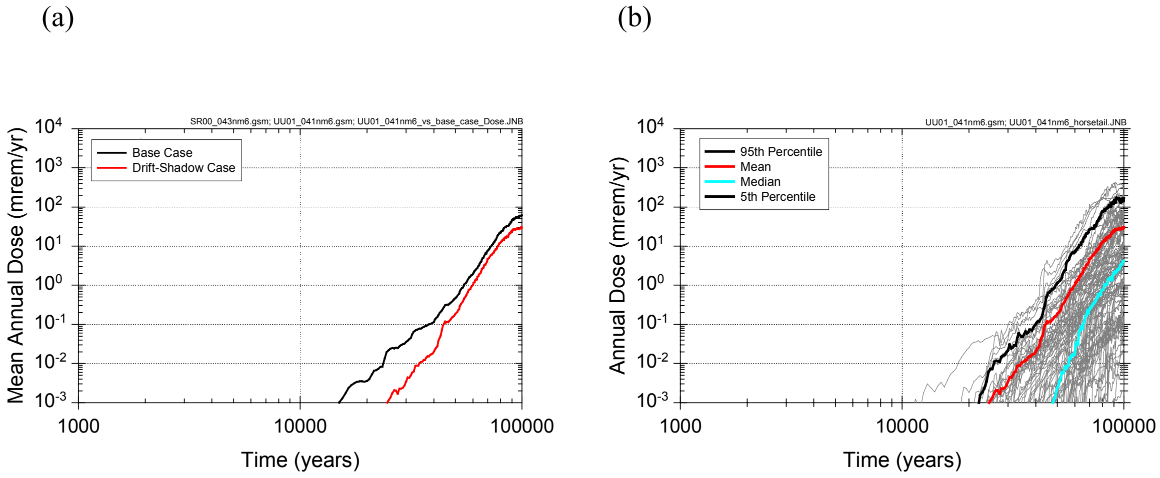

Fig. 3. UZ drift shadow sensitivity case: (a) Comparison of mean annual dose between the SSPA drift-shadow model and the TSPA-SR base case model; and (b) Range of results for all 100 realizations of the mean annual dose history for the new SSPA drift shadow model.

SUPPLEMENTAL TSPA MODEL

This section documents results of supplemental TSPA analyses conducted using a modification of the TSPA-SR model that incorporates many new models and input parameter values. These modifications have been made based on insights from uncertainty analyses discussed above and on new information developed since completion of the TSPA-SR, as described in SSPA Volume 1 (3). Model and parameter changes for the supplemental TSPA model are described in detail in SSPA Volume 1 (3) and summarized below.

Supplemental Climate Model–The supplemental TSPA model is updated to include climate changes after 10,000 years in the future. The updated climate model continues the current climate model until 38,000 years, when a full glacial period begins. The next full glacial period begins at 106,000 years in the updated model. Full glacial periods are anticipated to be 8,000 to 40,000 years in duration, and recur approximately every 90,000 years on average. The repository-average net infiltration for the full glacial states ranges from 17 millimeters per year (mm/yr) to 110 mm/yr. Interglacial climates represent present-day conditions. Intermediate climates are also represented in the model and are equivalent to the glacial-transition climate of the TSPA-SR model.

Supplemental Seepage Model–The seepage model is changed to reflect new seepage data for the Topopah Spring lower lithophysal hydrogeologic unit, in which most of the potential repository would be located. Previously, seepage data were only available for the Topopah Spring middle nonlithophysal unit. These new data indicate that the seepage threshold (the percolation flux above which seepage occurs) is higher in the lower lithophysal unit than in the middle nonlithophysal unit. The revised seepage abstraction takes into account differences between the units by developing distributions of uncertainty and spatial variability separately for the lithophysal and nonlithophysal units. To do so, the two sets of results are combined and weighted by the fraction of the repository in each rock type: (1) approximately 80 percent in the lithophysal unit; and (2) 20 percent in the nonlithophysal unit. Inclusion of results for the lower lithophysal unit, with its higher seepage threshold, results in lower estimates of the seepage fraction (the fraction of waste-package locations with seepage) in the revised seepage abstraction.

Supplemental Seepage Flow Focusing Model–The updated distribution of the flow-focusing factor for seepage is based on simulations of unsaturated-zone flow that were performed using heterogeneous permeability fields. The resulting flow enhancements are not as large as in the original model, usually less than a factor of 3 and always less than a factor of about 6. The flow-focusing factor is exponentially distributed, with a minimum focusing factor of 1 and a mean focusing factor of 2. Because of the lower degree of flow focusing, the average seepage rate in the regions that have seepage is lower than in the original model by nearly a factor of 10. At the same time, approximately 50 percent more waste packages are exposed to seepage.

Supplemental Model for Episodic Seepage–Episodicity in seepage induced by accumulation and subsequent release of water at fracture asperities is accounted for by an episodicity factor, which is the fraction of time that flow occurs. The distribution of episodicity factors used for this sensitivity analysis is a log-uniform distribution between 10^{-4} and 1. This factor increases the mean seepage rate during the time seepage occurs.

Supplemental Model for Thermal Properties–The model for thermal properties of the host rock has been updated to integrate new information obtained for the Topopah Spring lower lithophysal unit. In addition, thermal properties of the drift invert are updated to take into account the effects of carbon steel in the invert. These changes result in small changes to the temperature in the host rock and in the emplacement drifts and in the relative humidity in the emplacement drifts. Because changes in thermal properties may affect multiple components of the modeling system, these changes were not examined through one-off sensitivity analyses but rather through use of the supplemental TSPA model (see Fig. 4).

Supplemental Model for Thermal Hydrologic Effects on Seepage–The model is modified to take into account the changes in the thermal properties discussed above. In addition, the model is modified to incorporate direct effects of higher temperatures on seepage into the emplacement drifts. The model used in this case is less extreme. In this case, when the temperature at the drift wall exceeds 96ºC, the seepage is multiplied by a reduction factor between 0 and 0.2. The factor is distributed uniformly between these two values.

Supplemental Model for In-Drift Chemistry–The supplemental TSPA model utilizes better-constrained thermodynamic and kinetic data to improve the representation of the ambient water chemistry and the temperature dependence of that chemistry. The model also takes into account new information from the Topopah Spring lower lithophysal unit to provide a more representative host rock mineralogy; in particular, it includes contributions from fluorides not considered previously. The supplemental TSPA model also improves the representation of evolution of solids and water during the thermal period due to evaporation of water occurring in the emplacement drifts. In the low humidity range, bounding simplifications are used to overcome limitations in the model formerly used to make the estimates.

Supplemental Model for Stress Corrosion Cracking (SCC) of Alloy 22–The modified SCC model takes into account four changes. The first is a changed representation for the fraction of the weld flaws that can propagate. The supplemental TSPA model provides an updated estimate of this fraction. The second change addresses repassivation at the SCC crack tip. The new model is based on new information for Alloy 22 (the corrosion-resistant nickel-chromium-molybdenum metal alloy used for the outer layer of the waste packages). The third change is in the representation of uncertainty in the residual stress profile for the closure welds region of the outer waste package barriers. The representation makes use of updated values for the upper bounds of the uncertainty distributions. The fourth change is an updated distribution of the threshold stress for crack initiation. The new representation provides an updated probability distribution.

Supplemental General Corrosion Model–The supplemental TSPA model takes into account temperature dependence of the general corrosion rate of the Alloy 22 outer waste package barrier. This temperature dependence is developed from potentiostatic polarization tests (3). In addition, the uncertainty in the degradation due to general corrosion is assumed to be due entirely to uncertainty in the corrosion process itself and not to variability in conditions or structure.

Supplemental Model for Early Failure of the Waste Package–The supplemental TSPA model includes an increased probability for early waste package failure due to improper heat treatment (induction annealing) of the closure lid welds.

Supplemental Model for Evaporative Reduction of Seepage–A model for evaporative reduction of seepage through the EBS is included in the SSPA supplemental TSPA model.

Supplemental Model for Geometrical Constraints on Flow through the Waste Package–The supplemental TSPA model takes into account the fact that breaches in the drip shield may not occur directly over breaches in the waste package and that flow through the drip shield may not all enter the waste package.

Supplemental Model for In-Package Chemistry–The supplemental TSPA model has been modified to take into account the effect of waste form and iron degradation products on the in-package chemistry.

Supplemental CSNF Cladding Degradation Model–The supplemental TSPA model incorporates new probability distributions for creep rupture and stress corrosion cracking parameters, for localized corrosion, and for cladding unzipping. In addition, ranges for failures due to rockfall and for the frequency of seismic events are taken into account.

Supplemental Model for In-Package Radionuclide Solubility Limits–As previously discussed, the supplemental TSPA model is modified to increase the range for the uncertainty in the effect of the controlling mineral phases for plutonium, neptunium, and thorium.

Supplemental Model for Diffusive Transport within the Engineered Barrier System–As previously discussed, the supplemental TSPA model is modified to include a component for diffusive transport through thin films on the surface of in-package components. The model for the diffusivity of the drift invert is also updated.

Supplemental Model for Radionuclide Sorption within the Engineered Barrier System–As discussed in the previous section, the supplemental TSPA model includes the effect of sorption within the waste package and in the drift invert. The model explicitly represents sorption partition coefficients (K_ds) for corrosion products and other materials within the waste package and drift invert.

Supplemental Model for Radionuclide Transport in the Unsaturated Drift Shadow Zone–As discussed in the one-off sensitivity section, the transfer of radionuclides from the EBS to the UZ uses a modified representation of diffusive and advective flux releases. Diffusive EBS releases are transferred to UZ matrix transport rather than to fracture transport.

Supplemental Model for Radionuclide Transport in the Saturated Zone–The supplemental TSPA model uses a modified representation of the bulk density of the alluvium. In addition, the sorption coefficients for iodine and technetium have been changed to zero in the alluvium to reflect new experimental data.

Supplemental Biosphere Dose Conversion Factors–The supplemental TSPA model includes modified information regarding the biosphere dose conversion factors for key radionuclides.

Calculation Method

The TSPA model, which is encoded with the GoldSim computer code (6), can be run in a single-realization mode, which is sometimes done in order to conduct an in-depth examination of a particular realization. However, the model is normally run in a multiple-realization probabilistic mode so that effects of uncertainty can be analyzed. Since each realization of a multiple-realization simulation is independent from the others, GoldSim can run on a network, with multiple realizations computed simultaneously on as many processors as are available. This feature greatly facilitates probabilistic simulation of the complex TSPA model, in which a single realization can take hours to complete.

The three primary sets of TSPA simulations shown here are the base-case TSPA-SR model (2), the supplemental TSPA model at the HTOM (4), and the supplemental TSPA model at the LTOM (4). The first two (base case and HTOM) simulate essentially the same potential repository design, but with a number of differences in the component models, as discussed above. The third (LTOM) uses the same component models as HTOM, but simulates a lower-temperature design (lower thermal loading and longer preclosure ventilation period).

Results

The results of the various TSPA simulations are extensively documented (2,4). Here there is only room to present a small subset of the available results. Fig. 4 shows a comparison of the nominal mean-dose results for the three cases: (1) the TSPA-SR base case; (2) the supplemental TSPA HTOM model; and (3) the supplemental TSPA LTOM model. It can be seen that the HTOM and LTOM results are quite similar, even though there is a considerable difference in temperature between the two at early times (peak HTOM waste-package temperature is on the order of 160ºC, whereas peak LTOM waste-package temperature is on the order of 80ºC). This result indicates only a weak temperature-dependence in the calculated dose. On the other hand, there is a large difference between the base-case results and the supplemental-model results. The most important model changes causing this difference are the following:

- Waste-package corrosion. There are several significant changes in the waste-package corrosion model from the base case to the supplemental model. The one that had the largest effect was the addition of temperature-dependence to the model for waste-package general-corrosion rate. In the supplemental model, as temperature declines over time the general-corrosion rate gets very low, and the result is that most waste packages take significantly longer to fail. Waste-package failure drives the dose results to a great degree, as is clear from a comparison of the two plots in Fig. 4a.

- Premature waste-package failures. The supplemental TSPA model includes a higher estimate of the probability that waste packages might be breached prematurely because of improper heat treatment of the welds. The premature failures lead to a low mean annual dose before 10,000 years, whereas the base case has no waste-package failures, and therefore no dose, before 10,000 years.

- Climate. The base-case TSPA model used a simplified climate model with no climate changes except in the first 2,000 years. The addition of a more realistic climate sequence to the supplemental TSPA model causes many spikes in its dose curves after about 100,000 years, while the base-case mean dose curve is smooth.

- Radionuclide mobilization and transport. There are several changes from the base-case model to the supplemental model related to radionuclide mobilization and transport, including changes in the distribution of seepage that enters emplacement drifts, reductions in solubility for some key radionuclides (most importantly, ^{237}Np), and inclusion of some transport effects that had previously been neglected (a model for diffusive transport on thin films inside waste packages, sorption of radionuclides in the waste packages and in the drifts, and release of radionuclides that diffuse out of the EBS into the matrix continuum rather than the fracture continuum for UZ transport).

The dose curves in Fig. 4a are just the means of the distributions of dose at each time. The entire dose distribution can be examined to determine how much uncertainty there is in the dose calculations. Two examples are given in Fig. 4b: (1) the distribution of doses at 10,000 years; and (2) the distribution of peak-dose values. The 10,000-year dose is of interest because the regulatory period is specified as 10,000 years. Peak dose is of interest because it represents the maximum risk from the potential repository. Note that the dose in many realizations of the supplemental TSPA model is still increasing at 1,000,000 years, so that the peak is actually not yet attained. It is evident from both Figs. 4a and 4b that the peak doses are much lower in the supplemental TSPA model than in the TSPA-SR model. This is partially due to the lower rate of waste-package failures and partially due to other model changes, such as the reduction in estimated solubility for some radionuclides.

It is also useful to know which radionuclides are the greatest contributors to the calculated dose. At early times (the first 60,000 or 90,000 years) the dose is dominated by the highly soluble, very mobile radionuclides, Carbon-14 (^{14}C), ^{99}Tc, and Iodine-129 (^{129}I). After that, the dose is dominated by ^{237}Np, with increasing contributions by several other actinides at late times (Protactinium-231 [^{231}Pa], Radium-226 [^{226}Ra], Actinium-227 [^{227}Ac], Plutonium-242 [^{242}Pu], Thorium-229 [^{229}Th], Thorium-230 [^{230}Th], Lead-210 [^{210}Pb]).

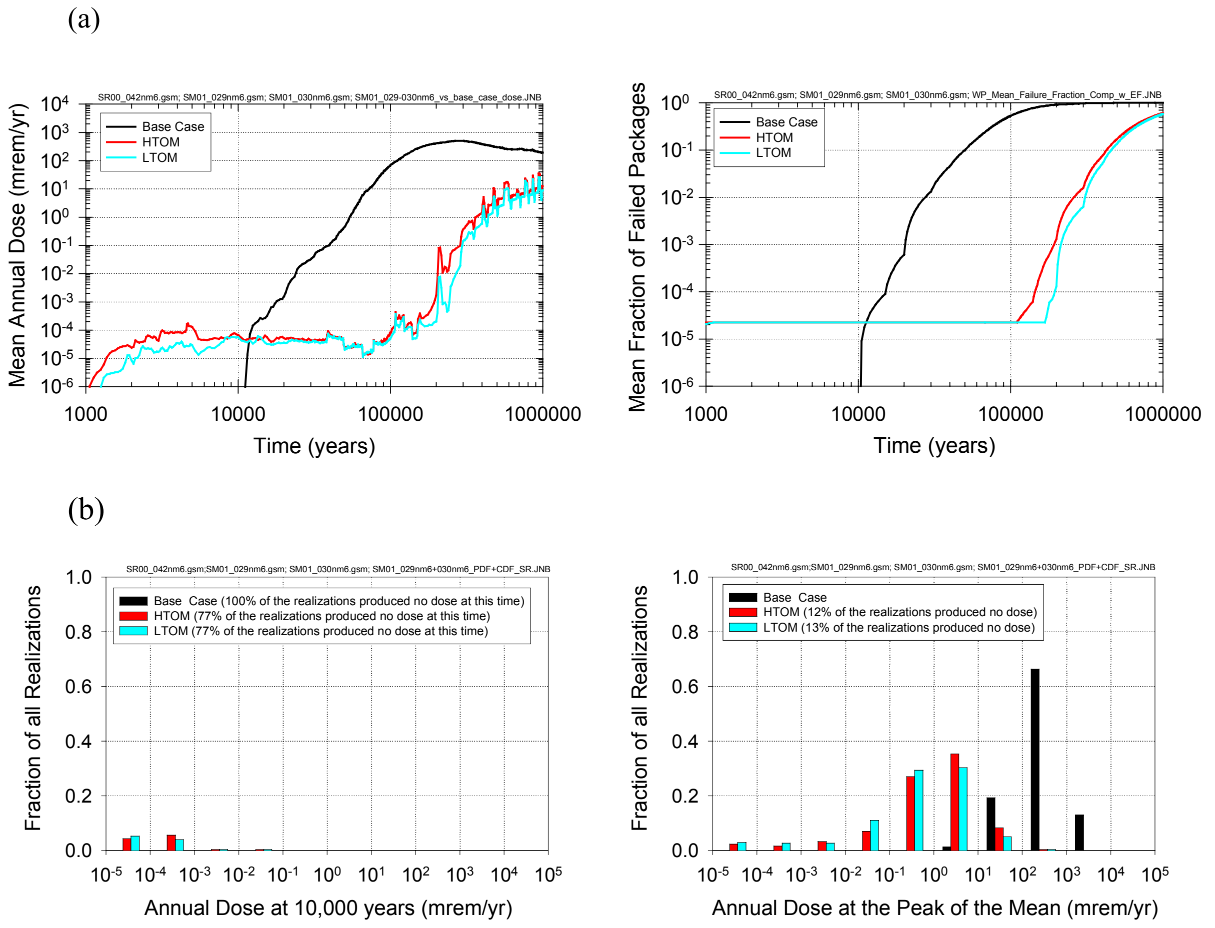

Fig. 4. (a) Mean annual dose (left) and mean fraction of waste packages failed (right) versus time for the nominal-scenario simulations (based on 300 realizations); and (b) histograms of dose at 10,000 years (left) and peak dose within 1,000,000 years (right) for the nominal-scenario simulations.

CONCLUSIONS

Comparisons at the system and subsystem levels (Fig. 4) between the TSPA-SR model and the supplemental TSPA model provide insight into the ways that uncertainties have been addressed and quantified. Likewise, the one-off sensitivity analyses (Figs. 1 to 3) provide information regarding the potential effects of the uncertainties and supplemental TSPA models on performance at an individual process model level. The following general conclusions have been reached regarding the overall significance of the quantified uncertainties and model updates.

Comparison of dose histories over 1,000,000 years for the TSPA-SR base-case and the SSPA supplemental TSPA model shows the following two characteristics. First, the supplemental TSPA model shows significantly wider ranges of doses at any given time and a wider range of times to reach any given dose value. Second, except at early times, the magnitude of the dose rate is less for the supplemental TSPA model and it occurs later in time. The broader range is a result of the additional uncertainties and updated models that have been incorporated into the SSPA supplemental TSPA model. In many cases, simplified or bounding models have been replaced with more physically representative models that include quantified uncertainties in their parameters. For example, a bounding solubility model for neptunium in TSPA-SR has been replaced with a more complex model that accounts for the solubility of secondary phases that control the solubility. The updated solubility model is believed to be more realistic, but the uncertainties in the model lead to a broader range of neptunium concentrations than the previous model. Propagation of these uncertainties, as well as those of all of the other updated process models, results in the broad ranges that are seen in results of the SSPA supplemental TSPA model (Fig. 4b).

The second observation is based on a comparison of the estimates of mean performance (dose rate and time to dose) for the TSPA-SR case and the SSPA supplemental TSPA cases, which shows that after approximately 10,000 years the mean annual dose for the supplemental TSPA model is always less than the mean for the TSPA-SR model. The difference between the mean estimates is one measure of the magnitude of the conservatism in the TSPA-SR model. For example, at 30,000 years, the difference between the mean estimates of dose rate is about three orders of magnitude (Fig. 4a), and at time of peak mean dose the difference is about one order of magnitude (Fig. 4a).

During the period prior to 10,000 years, the small mean annual doses (less than about 0.0002 millirem/yr) indicated by the supplemental TSPA model clearly exceed the zero annual doses calculated in TSPA-SR, and the supplemental TSPA model could be interpreted as being nonconservative with respect to the TSPA-SR model during this time. However, these small doses, resulting from the revised treatment of uncertainty regarding the potential for improper heat treatment of lid welds on waste packages, are more than a factor of ten thousand below applicable regulatory limits. Differences between the supplemental TSPA model and TSPA-SR have essentially no impact on conclusions that might be drawn with respect to comparisons with quantitative regulatory limits.

From the standpoint of uncertainties at the total system level, the supplemental TSPA model HTOM and LTOM cases show essentially comparable nominal performance, and both are significantly different from the TSPA-SR model. The small differences between the HTOM and LTOM are mostly due to the temperature dependency of the general corrosion rate for the waste package, resulting in lower corrosion rates for the LTOM.

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