15. SUMMARY AND CONCLUSIONS

The *FY01 Supplemental Science and Performance Analysis, Volume 1: Scientific Bases And Analyses* Report (SSPA) describes new information developed since completion of the *Yucca Mountain Science and Engineering Report* (S&ER) (DOE 2001 [DIRS 153849]), and its key references, the *Total System Performance Assessment for the Site Recommendation* (TSPA-SR) (CRWMS M&O 2000 [DIRS 153246]), and the Analysis and Model Reports and Process Model Reports cited therein. Volume 1 (BSC 2001 [DIRS 154657]) describes the new technical work at the process model level. The *FY01 Supplemental Science and Performance Analysis, Volume 2: Performance Analyses* (McNeish 2001 [DIRS 155023]) describes analyses conducted to gain insight into the implications of the new technical work on the performance of the potential repository.

The analyses described in this report were performed to address uncertainties that were acknowledged in the S&ER (DOE 2001 [DIRS 153849]). As described in Section 4.1 of the S&ER (DOE 2001 [DIRS 153849]), the DOE approach to accommodating uncertainty includes a quantitative analysis of performance, supplemented by several additional measures designed to independently provide confidence that the quantitative models are defensible. The additional measures include the selection of a site and design of a repository system that provides defense in depth and a margin of safety compared to requirements, insights obtained from natural and man-made analogues, and a commitment to a long term performance confirmation, management and monitoring program.

Although the S&ER (DOE 2001 [DIRS 153849]) and its key references include substantial discussions of uncertainty, the DOE determined that additional work to augment the characterization and treatment of uncertainty was warranted. Therefore, several types of analyses were identified and performed to supplement the treatment of uncertainty in support of the consideration of a possible site recommendation. The supplemental information can be divided into three areas:

- **Unquantified Uncertainties Analysis**–Some of the uncertainties that were not quantified in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) have been quantified. Newly quantified uncertainties include updates to parameter bounds, conceptual models, assumptions, and in some cases, statistically biased or skewed distributions on input parameters. The primary goals of this portion of the effort were to provide insight into the importance of the unquantified uncertainties and the degree of conservatism in the overall assessment of the performance of the potential repository presented in TSPA-SR (CRWMS M&O 2000 [DIRS 153246]).

- **Updates in Scientific Information**–New information has been developed for the process models supporting the total system performance assessment (TSPA). This work includes new experimental results, new conceptual models, new analysis approaches, and the results of continued research efforts. 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 portion of the work were to provide insights into the impact of the new scientific results and improved models (i.e., updated since completion of the S&ER (DOE 2001

[DIRS 153849])) and to develop additional confidence in the models and parameters used for TSPA.

- **Lower-Temperature Operating Mode Analysis**–The effects of a range of thermal operating modes (including lower operating temperatures in the potential repository) on projected system performance have been evaluated. Different thermal modes are compared with the design and operating mode described in the S&ER (DOE 2001 [DIRS 153849]). The primary goals of evaluating a range of thermal operating modes were to provide insights into the effect of thermal parameters on predicted repository performance, including uncertainty of those predictions, and to increase confidence in the predicted repository performance over a range of thermal conditions.

The SSPA provides information that can be used to assess the robustness of the analyses and results presented in the S&ER (DOE 2001 [DIRS 153849]). It also provides a technical basis for a preliminary evaluation of some of the advantages and disadvantages of alternative thermal operating modes for the potential repository. The new analyses described in Sections 3 through 14 of this volume are organized and presented by key system attributes and by process models, as they are defined in the S&ER (DOE 2001 [DIRS 153849], Table 4-3). Table 1-1 in Section 1 (Introduction) of this report shows the supplemental models and analyses that were performed for the SSPA, and the rationale for the analyses. The updated models and sensitivity analyses that were incorporated in the supplemental total system performance assessment models are described in Volume 2 (McNeish 2001 [DIRS 155023]) are identified in Table 1-1.

General Conclusions–The analyses described in the SSPA have enhanced the DOE understanding of the uncertainties inherent in assessments of the potential future performance of a Yucca Mountain repository. The quantification of uncertainties has improved the understanding of conservative and potentially non-conservative assumptions contained in the process models described in the S&ER (DOE 2001 [DIRS 153849]) and its references. Depending on the process model, reductions in uncertainties can be obtained from either the lower-temperature operating mode (LTOM) or the higher-temperature operating mode (HTOM). The preliminary evaluation of thermal operating modes indicates that post-closure effects on performance can be evaluated by selecting appropriate initial conditions for the models. The analysis of waste package degradation indicates that performance models should consider the thermal dependence and the local chemical environment that control corrosion mechanisms and rates. The expanded consideration of multiple lines of evidence throughout the SSPA is a useful exercise that has improved understanding by the DOE of processes important to repository performance, independent of the results of the quantitative TSPA.

Preliminary Comparison of Lower- and Higher-Temperature Operating Modes–The preliminary evaluations presented in the SSPA indicate that the process models used for the TSPAs for Yucca Mountain are appropriate for analyzing the LTOM and HTOM. The results of the analyses suggest that the differences between thermal operating modes are significant only for the first few thousand years after emplacement, because the thermal differences are negligible after the initial thermal pulse. This fact largely accounts for the similarity in postclosure performance results. Process model results indicate that natural processes (e.g., unsaturated zone flow above the repository, seepage into drifts, and flow and transport in the unsaturated and saturated zones below the repository) are not significantly influenced over the long term by the thermal operating mode. Evaluation of coupled thermal-hydrologic-chemical-mechanical processes demonstrates that LTOMs have lesser (and less complex) effects on the processes operating in the thermally perturbed region near emplacement drifts, but also shows that the effects are generally small, and relatively short-lived, for higher-temperature modes. Process models representing the performance of the engineered barrier system components are sensitive to the physical (temperature and relative humidity) and chemical environment in the repository. However, the analyses also suggest that the relatively short duration of conditions in which drip shield or waste package corrosion may be possible is unlikely to result in significant degradation of performance. The analysis of varying operating modes indicates that a variety of design/operating mode parameters and configurations can be used to manage the thermal environment.

15.1 KEY ATTRIBUTE: LIMITED WATER ENTERING EMPLACEMENT DRIFTS

The processes that control the amount of water available to enter emplacement drifts in the potential repository are described in Sections 3 (Unsaturated Zone Flow) and 4 (Seepage) of the SSPA. Since the completion of the S&ER (DOE 2001 [DIRS 153849]), a variety of improvements to the unsaturated zone and seepage flow models have been made, and additional analyses have been undertaken to assess the possible effect of LTOMs on the uncertainties associated with the models. In particular, the LTOM analyses have addressed the coupled thermal-hydrologic-chemical-mechanical processes that influence the flow of water and the potential transport of radionuclides in the thermally affected region near emplacement drifts.

The results of the SSPA analyses generally indicate that the effects of the improved models on performance results are small, or that the assumptions used in the S&ER (DOE 2001 [DIRS 153849]) and the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) were conservative. In most cases, the effects of the improved models are less than the variability and/or uncertainty that was incorporated into the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). Similarly, the evaluations presented in the SSPA confirm that thermal effects on coupled hydrologic, chemical and mechanical processes on performance is less for LTOMs than for HTOMs. However, the differences between the HTOM and LTOM appear to be small for all of the processes analyzed.

The discussions that follow provide a brief synopsis of the SSPA results for each of the topics addressed:

Post-10,000-Year Climate Model–A post-10,000-year climate model has been developed for inclusion in supplemental TSPA analyses. The model of climate over the next 1,000,000 years incorporates alternating climate stages including intermediate, monsoon, interglacial, and three distinct full glacial stages. Each stage has been defined by a range of mean annual precipitation rates and temperatures. Full-glacial stages encompass about 21 percent of the next 1,000,000 years. Based on paleoecological and paleoclimatic records and analogue site data, the climate is expected to be cyclical within 400,000-year periods and the climate changes are assumed to relate to earth orbital precession and eccentricity parameters. The effect of the variable climate has been incorporated in the TSPA results presented in Volume 2 (McNeish 2001 [DIRS 155023]). Although the range of potential climates is broadly represented, uncertainties remain with respect to the timing, duration, and nature of climate changes over the next 1,000,000 years. Tectonic changes and other climate forcing functions (such as the rain shadow effect caused by uplift of the Sierra Nevada Mountains) have remained relatively constant during the past 1 million years and are expected to remain so for the next 500,000 years, but may impact future climate at the 1 million year time scale.

Infiltration Rates for the Post-10,000-Year Climate Model–The predictions of future climate, precipitation, and resulting infiltration rates show that as climate changes from interglacial (modern) to monsoon, to intermediate (glacial-transition) to glacial, the mean precipitation and infiltration rates also increase. Updated estimates of net infiltration for 10,000 years to 1,000,000 years in the future have been developed based on the precipitation rates and temperatures predicted for each future climate state. Relatively high net infiltration rates occur generally in the northern portion of the site at high elevations and along ridges where fractured bedrock is exposed. The uncertainty in net infiltration from imperfect knowledge of input parameters has been quantified for the intermediate (glacial-transition) climate, the dominant climate in the next 1,000,000 years. These results are included in the performance assessment analyses described in Volume 2 (McNeish 2001 [DIRS 155023]).

Flow in the Non-Welded Paintbrush Tuff (PTn)–Additional analyses of flow in the PTn have been developed to test simulation models by comparing their results to available data and revising the models where appropriate. These analyses included the use of chloride data to evaluate the distribution of net infiltration with isotropic permeability within the PTn; the use of a detailed two-dimensional model of the PTn to evaluate the importance of lateral flow due to capillary barrier diversion within the unit; and analyses developed to resolve the difference between the net infiltration distribution above the PTn and the calibrated net infiltration distribution below the PTn. The high matrix porosity and low fracture frequency in the tilted, non-welded PTn can effectively damp out episodic infiltration pulses and divert percolating water to the intercepting faults and fault zones. The evaluations also suggest that lateral flow within the PTn hydrogeologic unit may lead to a relatively uniform percolation distribution below the PTn. The relatively uniform percolation (which is consistent with observations and the chloride data) may reduce the variability and associated uncertainties in assessments of unsaturated zone waste-isolation capacities.

Three-Dimensional Flow Fields–New three-dimensional flow fields have been developed to support analyses of an expanded repository layout including a southern repository extension, further analyses of a steep hydraulic gradient near the northern end of the repository footprint, variable thickness of PTn and fault property uncertainty. Uncertainties in boundary conditions (especially the infiltration rates and distributions) and in rock properties contribute to uncertainties in the three-dimensional flow fields. Sensitivity and bounding studies were used to identify and quantify uncertainties. Unsaturated zone model results have been compared with data and evaluated to test the sensitivity of the model to processes, parameters, alternative conceptual models, and other numerical approaches. These evaluations indicate that the unsaturated zone model incorporates site characteristics and important processes in a manner that is consistent with observations and test results, providing confidence in the unsaturated zone flow model.

Effects of Lithophysal Porosities–The effects of lithophysal porosities on thermal properties were analyzed and indicate that the lithophysal cavities reduce the effective thermal conductivity and the thermal capacity of the matrix continuum in the upper-lithophysal (tsw33) and lower-lithophysal (tsw35) hydrogeologic units. For the same thermal load, explicitly accounting for the effects of lithophysal cavities leads to an increase in temperature caused by heat released over the same period. These updated properties have been incorporated in performance assessment analyses described in Volume 2 (McNeish 2001 [DIRS 155023]).

Mountain-Scale Thermal-Hydrologic Effects–The mountain-scale thermal-hydrologic models provide analyses of temporal and spatial variability in the unsaturated zone conditions under thermal loads. The S&ER (DOE 2001 [DIRS 153849]) describes an operating mode with an initial thermal load of 72.7 kW/acre (1.45 kW/m of drift), and a forced ventilation period of 50 years, during which 70 percent of the decay heat was assumed to be removed. To lower the drift wall temperature below the boiling point, a lower areal thermal load (67.7 kW/acre or 1.35 kW/m of drift), longer forced-ventilation period (300 years), and higher heat-removal efficiency (80 percent) are evaluated. Induced temperature changes have effects at drift walls, within the pillars, at perched water bodies, at the water table, and throughout the unsaturated zone system. The coupled thermal-hydrologic processes can change the extent of two-phase and dryout zones around the drifts, induce large liquid and gas flux in the near- and far-field environments, redistribute the moisture, and affect the drainage potential through the pillars. Thermal conductivity and heat capacity of the rock mass are modified to account for the lithophysal porosity in the tuff matrix properties. For the lower-temperature cases, the thermal-hydrologic models predict little change in unsaturated zone liquid flux except in the immediate vicinity of the potential repository drift. Because boiling conditions do not occur, and the fractures are not completely dry, the mountain-scale thermal-hydrologic model predicts reduced (but nonzero) flow crossing the repository horizon throughout the thermal-loading period (about 2,000 years). Uncertainties in the unsaturated zone flow system model contribute to uncertainties in the mountain-scale thermal-hydrologic processes.

Mountain-Scale Thermal-Hydrologic-Chemical Effects–The mountain-scale thermal-hydrologic-chemical model has been updated and used to evaluate how coupled thermal-hydrologic-chemical processes may affect rock properties and flow and transport processes at the mountain or potential repository scale. The updated model incorporates new thermodynamic and kinetic parameters, calibrated against drift-scale heater tests, and water chemistry data from matrix pore water collected near the ongoing drift-scale test. Temperature dependent processes such as condensation and dryout/boiling have been analyzed, as have the effects of elevated temperatures on reaction rates and the thermodynamic stabilities of minerals. The updated analyses have also considered the effect on pH, mineral-water reactions, and reaction rates caused by the release of carbon dioxide out of water and transport in the gas phase via advection and diffusion. Uncertainties in flow processes (including gas convection, liquid flow focusing, and diversion) and data have been studied. Data uncertainties analyzed include thermodynamic and kinetic data of vitric and zeolitic tuffs, precipitating mineral assemblages, effective mineral-water reactive areas in heterogeneous unsaturated fracture rocks, fracture and lithophysal hydrologic properties, and distributions of water and gas chemistry in the unsaturated zone and in the infiltrating water. Sensitivity studies were conducted to understand the impact of thermal-hydrologic-chemical processes on mineral changes during thermal periods in the zeolitic CHn, on matrix porosity reduction in the TSw, on enhanced precipitation at the edges of the potential repository block with gas convection, and on many other thermal-hydrologic-chemical effects. These analyses indicate that the effect of thermal-hydrologic-chemical processes such as mineral precipitation and dissolution on hydrologic properties and percolation flux are not significant compared to the changes in flow processes and rates caused by the thermal-hydrologic effects described above. The overall range in chemistry is comparable to that observed in previous analyses. The ranges in pH of about 7 to 9 are strongly linked to changes in gas-phase carbon dioxide concentrations. In the center of the repository, pH tends to be higher (and carbon dioxide lower) than near the edges of the repository.

Mountain-Scale Thermal-Hydrologic-Mechanical Effects–A new coupled thermal-hydrologic-mechanical model was developed to calculate the impact of thermal-hydrologic-mechanical processes on flow at the mountain scale. The mechanical behavior of porous and fractured media responds to changes in temperature, in effective stress, and in strain, resulting in permeability, porosity, and flow-field changes. The model results indicate that mountain-scale changes to hydrologic properties are moderate. Nevertheless, uncertainties in the thermal-hydrologic-mechanical model contribute to uncertainties in the thermal-hydrologic model, and further work is ongoing to build confidence in the models.

Effect of Flow-Focussing on Seepage–Analyses were conducted to investigate flow-focussing within the heterogeneous permeability field and the effects of episodic infiltration. The studies used a stochastic fracture continuum model to evaluate flow focusing through fractures from the bottom of the PTn to the potential repository horizon. These studies were carried out using a 100-m wide and 150-m deep two-dimensional cross section covering the upper five TSw hydrogeological units at Yucca Mountain. Heterogeneous fracture permeability distributions were generated using a stochastic approach conditioned on field-measured air-permeability data. The studies considered various percolation fluxes, correlation lengths, and uniform and nonuniform percolation-flux boundary conditions. The results provide a quantitative analysis of flow focusing. All simulation results indicate that the flow focusing factor is likely to be much smaller than the value used in previous TSPA calculations (CRWMS M&O 2000 [DIRS 153246]); therefore, the TSPA calculations are conservative with respect to flow focusing issues, since they use a flow focusing factor that may be an order of magnitude higher than that suggested by the new studies. In addition, the sensitivity analyses indicate that frequency distributions of normalized flux are insensitive to the magnitudes or spatial distributions of percolation fluxes specified on the upper boundary or to the spatial correlation structure of the permeability fields within the unsaturated zone.

Effects of Drift Degradation and Rock Bolts on Seepage–Drift degradation and the impact of rock bolts were investigated in order to quantify uncertainty in seepage rates associated with those processes. The studies indicate that there is no significant enhancement of seepage caused by intact or degraded rock bolts, and that rock bolts may be neglected as a seepage-enhancement factor for performance assessment. The studies also indicate that seepage enhancement due to drift degradation processes is relatively small (on the order of 0 to 5 percent).

Thermal-Hydrologic Effects on Seepage–Thermal effects on seepage were examined through a modeling study that assessed model uncertainties regarding grid resolution and heterogeneity. The study also examines the impact of lithophysal cavities on thermal properties, the potential for liquid water to penetrate superheated region, causing episodic seepage events, and the development of a vaporization barrier. Moreover, percolation flux was calculated for a range of thermal operating modes.

The updated model considered thermal expansion as well as dissolution and precipitation of minerals that could lead to changes in fracture aperture and fracture coatings, potentially affecting the unsaturated hydrogeologic properties, fracture-matrix interaction, and the flow of liquid water or water vapor near drifts. Conceptual and parametric uncertainties in the model have been examined through extensive sensitivity analyses. These studies suggest that the simplifying assumptions contained in the seepage abstraction for performance assessments are conservative (i.e., they yield seepage estimates that are higher than the process model results).

Thermal-Hydrologic-Chemical Effects on Seepage–Thermal-hydrologic-chemical processes may impact seepage through thermally induced changes in unsaturated hydrogeologic properties. Additional validation studies were performed, enhancing the confidence into the thermal-hydrologic-chemical modeling approach. Sensitivity analyses were performed, examining different in-drift designs, different, heterogeneous host rock units, different systems of components and minerals, different kinetic models for mineral-water interactions, different permeability-porosity relations during precipitation and dissolution, and changed thermodynamic data and initial conditions. All these studies helped reduce conceptual uncertainties in the thermal-hydrologic-chemical models. Additional studies of coupled processes were performed for an extended range of temperatures, covering various thermal operating modes. The evaluations indicate that thermal-hydrologic-chemical effects on flow are small compared to the ambient variability around emplacement drifts for the HTOMs, and even smaller for the LTOM.

Thermal-Hydrologic-Mechanical Effects on Seepage–In support of the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), a distinct-element analysis was performed to examine thermal-mechanical effects of drift excavation and repository heat on hydrogeological properties. This analysis has now been revised and extended to provide a more robust estimate of thermal-mechanical effects in fracture permeability. The evaluations indicate that thermal-hydrologic-mechanical effects on flow properties are small compared to the ambient variability around emplacement drifts for the HTOMs, and even smaller for the LTOM. In addition, a fully coupled thermal-hydrologic-mechanical continuum model was developed and calibrated against air-permeability data from three niches and the Drift Scale Heater Test area. The successful calibration increased confidence in the conceptual model and reduced uncertainties in the subsequent prediction runs, which included two thermal operating modes.

15.2 KEY ATTRIBUTE: LONG-LIVED WASTE PACKAGE AND DRIP SHIELD

The processes affecting the life span of the drip shield and waste package in a potential repository are described in Sections 5 through 8 of this volume of the SSPA. Important processes include the water diversion performance of the engineered barriers, the distribution of moisture within the drifts, and drip shield and waste package degradation performance, which are a function of the physical (temperature and relative humidity) and chemical environment within the drifts. The SSPA describes a variety of analyses undertaken primarily to quantify some of the uncertainties in the analyses described in the S&ER (DOE 2001 [DIRS 153849]), and to assess the impact of a LTOM. In general, although the uncertainties are significant, the results of the analyses suggest that the representations of processes included in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) and the S&ER (DOE 2001 [DIRS 153849]) are conservative.

The effects of numerous processes and properties on water movement, in-drift physical and chemical environment, and drip shield and waste package performance were addressed through extensive sensitivity and uncertainty analyses presented in the SSPA. These evaluations indicate that models of the physical environment in the drifts (e.g., temperature and relative humidity) are sensitive to the thermal properties of the rock mass, especially lithophysal porosity, and to some of the operating mode variables that can be used to manage the thermal environment, such as the efficiency of ventilation in removing heat. Differences between alternative thermal models have been examined.

Corrosion and degradation rates for drip shields and waste packages are also sensitive to the chemical environment in the drifts, which can be affected by the composition of dust in the underground environment, as well as the chemical composition of seepage waters that may contact the engineered barriers. The evolution of water chemistry as fluids evaporate in the drift also affects the potential for degradation.

A model for early failures of waste packages has been developed and included in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). This non-mechanistic model is based on a scenario in which improper heat treatment leads to the early failure of a small fraction of waste packages. In contrast, the inclusion of temperature dependence in degradation models has a significant positive effect on long-term assessments of waste package performance. Reduced corrosion rates associated with declining temperatures after the first few thousand years may result in increased package lifetimes, and improved performance compared to the models used for the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]).

Overall, the analyses indicate little difference between LTOMs and HTOMs for waste package performance. The reason for the similarity is that few packages fail during the first few thousand years in either case. Waste packages emplaced in a LTOM repository would not experience physical (temperature, relative humidity) or chemical conditions favorable for corrosion. Waste packages emplaced in a HTOM may experience physical conditions in which crevice corrosion could occur for up to a few thousand years, but the aggressive chemical conditions necessary for crevice corrosion are not likely to occur.

Multiscale Thermal-Hydrologic Model, Including Effects of Rock Dryout–The multiscale thermal-hydrologic model was updated to incorporate improved representations of the thermal processes affecting flow in and near emplacement drifts, and to assess the effect of LTOMs on repository performance. Temperature-humidity conditions on typical pressurized water reactor waste package surfaces were analyzed for the HTOM and LTOM cases. All geographic locations (edge, corner, and center) were included for the two operating modes. Temperature-humidity conditions progress over time, ending at ambient conditions of about 25°C and 100 percent relative humidity. The LTOM results in lower relative humidity for any given temperature, or lower-temperature for any given relative humidity for most locations. The range of temperature-humidity conditions over time was compared to the environmental conditions in which Alloy-22 may be susceptible to initiation of crevice corrosion. As defined in the SSPA, this region of susceptibility is more conservative than that defined within the *License Application Design Selection Report* (CRWMS M&O 1999 [DIRS 103955], Figures 5-18, 5-32 and 6-1). Based on the deliquescence point of sodium nitrate, and the conservative assumption that stress corrosion cracking can occur in an environment which would sustain a stable water film, the region of susceptibility is defined by a lower temperature of between 85°C and 90°C and by relative humidity of 20 to 70 percent (determined by which salts may be present on the waste package surface). LTOM waste packages are nearly always at temperatures below the window of crevice corrosion susceptibility. In contrast, the HTOM waste package corrosion analyses must include evaluation of crevice corrosion for at least 3,000 years after emplacement when the temperatures drop to below 80°C.

Sensitivity to Thermal Property Sets, and Effect of In-Drift Convection on Temperatures, Humidities, Invert Saturations, and Evaporation Rates–Analyses were conducted using submodels of the multiscale thermal-hydrologic model to consider the sensitivity to operational parameters and to the uncertainty and variability of properties of the natural and engineered systems. These analyses considered the HTOM and the LTOM. The focus was on the effects of heat-driven coupled-processes on in-drift thermal-hydrologic conditions. The environmental conditions considered include temperature and relative humidity at the waste packages and drip shield, and saturation at the drift wall and in the invert.

Peak temperatures at the drip shield and waste package were most sensitive to ventilation parameters and to thermal conductivity used in the models. The uncertainty in host rock thermal conductivity had the most significant effect. The drift wall and drip shield peak temperatures had a range of 85 and 20°C (for the HTOM and LTOM) resulting from a thermal conductivity range of 1.13-2.01 W/m•K (saturated) and 0.54-1.54 W/m•K (dry). The key factor determining the spatial variability of thermal conductivity is the variability of lithophysal porosity. The range of drift wall and drip shield temperatures was about 100 and 25°C (for the HTOM and LTOM) when a range of 0 to 25 percent of lithophysal porosity was used. The increase in temperature was due to the additional effect of porosity on heat capacity, in addition to the effect on thermal conductivity.

The second most significant factors were those related to ventilation. There was a range of about 60°C (for the HTOM and LTOM) in pre-closure peak drip shield temperatures resulting from using constant versus time-dependent ventilation efficiency. A 14° and 7°C postclosure drip shield temperature range (for the HTOM and LTOM, respectively), resulted from a 20 percent variation in ventilation efficiency (heat removal). For the LTOM, it was concluded that a 44-year variability in ventilation duration from one part of the repository to another would have only a minor effect on postclosure temperatures.

The important uncertainties resulting from using two-dimensional analyses were also quantified. The detailed three-dimensional analyses of in-drift thermal-hydrologic effects calculated 26° and 8°C ranges (for the HTOM and LTOM, respectively) in postclosure peak temperatures from the hottest to the coolest waste packages.

The ventilation efficiency was calculated using two independent models, and compared to the quarter-scale tests. The models, which used a wide range of convective heat transfer coefficients, bracketed the measured results. The influence of water entering the drift and evaporating into the dry ventilation air was not significant on overall ventilation efficiency, and had only a minor effect on ventilation air humidity.

A number of other parameters were investigated, including the effect of lithophysal porosity on gas storage, seepage effects on in-drift humidity, imbibition hysteresis, buoyant gas-phase convection in the rock, thermal-hydrologic-chemical and thermal-hydrologic-mechanical processes, host rock permeability, invert conductivity, and treatment of thermal radiation and natural convection in the drift. These parameters had only small effects on the magnitude of in-drift temperatures. However, the invert conductivity and the sophistication of natural convection models were found to influence which part of the Engineered Barrier System are cooler than others, with potential influence on formation of condensate which could be the source for corrosion or transport.

Finally, multiple approaches to achieving LTOM temperatures were evaluated. Derating pressurized water reactor waste packages was the most effective method of reducing peak temperatures, followed by drift spacing (for line-loaded drifts), and finally, waste package spacing. However, the range of temperatures among these methods was small (within 3°C); therefore, other factors may determine the selection of a design/operating mode for the license application.

Composition of Water and Gas Entering Drift–Thermal-hydrologic-chemical seepage models were used to predict the composition of waters and gases that could enter potential waste emplacement drifts. Modeled thermal-hydrologic-chemical processes are complex, and the number and variability of model input parameters are large. For this reason, a rigorous quantification of model uncertainty is not achievable, and thermal-hydrologic-chemical modeling work performed to date has concentrated on limiting and qualitatively assessing uncertainty. Uncertainties affecting the predicted composition of fluids that could enter drifts were evaluated. These were related primarily to infiltration rates, thermodynamic and kinetic data, pore water and infiltration-water compositions, boundary carbon dioxide partial pressures, potential repository thermal operating modes, and potential repository host rock units. Input thermodynamic and kinetic data were identified as some of the main model uncertainties. These uncertainties can be minimized by model validation and calibration against field and experimental data. In such case, the uncertainty in initial and infiltration water compositions input into the thermal-hydrologic-chemical seepage models may overwhelm other model uncertainties. Relative to the variability in possible model input water compositions, predicted water compositions were not very sensitive to the investigated ranges of boundary carbon dioxide partial pressures, repository host rock units, or infiltration rates. The largest predicted effect of thermal loading on water compositions was decarbonation through volatilization of carbon dioxide. This is a common heating effect observed in natural geothermal systems. However, carbon dioxide concentrations in fractures around the drift are not predicted to reach high values (typically less than 4,000 ppmv). Higher-temperatures increase the variability of predicted concentrations at the drift wall, relative to lower temperatures. However, heating effects are predicted to be relatively short-lived. As temperatures decrease and return to ambient values (within 100,000 years), the predicted water compositions at the drift crown return to ambient values. At large liquid saturations around the drift (which would be most favorable to water-rock interaction and potential seepage into the drift), no extreme pH or salinity values were predicted.

Evolution of In-Drift Water Chemistry–The in-drift chemical environment was evaluated for uncertainty while attempting to provide more consistency between process model outputs supporting the TSPA analyses. Three submodels are used in the uncertainty analyses: the precipitates/salts model, the microbial communities model, and the in-drift (applied in the invert) water mixing model. All three of the submodels integrate geochemical inputs (e.g., water fluxes and chemical compositions) in a more consistent manner than prior calculations while supporting the TSPA.

- **Precipitates/Salts Model**–This model extends a model of brine concentration to combinations of chemical concentration and composition for which few calculations have been effective in the past. This allows quantitative prediction within validation criteria of the kind of solutions or salt precipitates that are available for metallic corrosion and geochemical interaction in the drift. Model validation has demonstrated that given accurate inputs for starting water and gas compositions, the precipitates/salts model will likely provide results that are within a factor of two for chloride concentrations and ionic strength and within a pH unit for pH predictions.

- **Microbial Communities Model**–This model provides bounding estimates through time of the numbers of potential microbes that could grow in the repository drift, while evaluating uncertainty from: drift temperature, relative humidity, water chemical concentrations, gas fugacities, and the percolation flux through time. Current model output indicates few significant changes compared to TSP SR (CRWMS M&O 2000 [DIRS 153246]), because of the conservative assumptions formerly employed.

- **In-Drift Water Mixing Model**–This model is designed to mix three different chemical solutions with differing water fluxes (crown, invert, and waste package) to determine the mixed solution pH, and ionic strength. At the same time, the in-drift water mixing model is used to evaluate the uncertainty from the percentage of fluid leaked from waste packages that mixes with other water sources in the invert. Such analyses indicate waste package leaking must be hundreds of times greater than presently calculated at the 50,000 year time step in the TSPA to produce mixed acidic waters which can enhance transport of radionuclides. These three submodels are used to determine the chemical conditions, over thousands of years up to a million years, that are used for the calculation of radionuclide releases from the Engineered Barrier System.

Thermal-Hydrologic-Chemical Model Comparison to Plug Flow Reactor and Fracture Plugging Experiment–Thermal-hydrologic-chemical simulations of a plug-flow reactor tuff dissolution experiment were performed. Using the same thermodynamic and kinetic data, as well as the same rock mineralogy and geochemical components as those used in the thermal-hydrologic-chemical seepage models, these simulations yield relatively good agreement between measured and predicted water compositions. Although the length of the modeled experiment (two months) is likely too short to fully assess the uncertainty of the thermal-hydrologic-chemical seepage model over thousands of years, this work improved the confidence in the thermal-hydrologic-chemical seepage models and their input thermodynamic and kinetic data.

Effects of Fracture Size and Spacing on Drift Degradation–The uncertainties associated with the extent of fracture planes and the spacing of subhorizontal joints in the rockfall model have been analyzed. The quantification of these uncertainties provides additional confidence that the model for rockfall can adequately predict the size ranges and quantities of rock that may fall into emplacement drifts. The sensitivity analyses for the rockfall model presented in this report confirm the appropriateness of the analysis parameter selection in the *Drift Degradation Analysis* (CRWMS M&O 2000 [DIRS 151635]). These sensitivity analysis results indicate no impact to the repository subsystems potentially affected by rockfall.

Evaporation of Seepage Contacting the Drip Shield–The heat contained in the waste package has the potential to evaporate a portion of in-drift seepage that might contact the drip shield. An updated model provides an estimate of the fraction of this heat needed to evaporate seepage as it contacts the drip shield. Drip shield evaporation depends on a number of parameters: waste package heat evolution, forced air ventilation of the preclosure period, natural ventilation during the postclosure period, and drip shield surface conditions. More evaporation will occur in the HTOM. The updated process model is based upon a flow splitting algorithm that included flux into breaches and away from breaches in the drip shield. No credit is taken for potential evaporation at the surface of the drip shield. Consideration of this process potentially reduces the amount of seepage available for transport through the Engineered Barrier System. Alternative thermal operating modes are addressed by assuming two different temperature and relative humidity distributions for the HTOMs and LTOMs. The impact on the amount of seepage available for transport over the range of thermal operating modes can be inferred from the time histories of time-dependent fluxes through the Engineered Barrier System (drip shield, waste package, and invert).

Condensation Under Drip Shields–This updated model quantifies the condensate flux on the underside of the drip shield due to evaporation and addresses what fraction will fall on the waste package. The model was developed for the original Engineered Barrier System flow abstraction, but was not included in subsequent calculations. This activity is only meant to supplement the rationale for screening out this process due to low consequence. Alternative thermal operating modes do not affect the conceptual model for condensation on the underside of the drip shield and waste package.

Effect of Breached Drip Shields or Waste Packages–The waste package degradation model provides for predictions of the type, number, and timing of breaches in the drip shield and waste package. This information is used by the Engineered Barrier System water diversion abstraction to define the time-dependent fluxes that flow through (or are diverted around) the drip shield and the waste package. In this model, droplets fall randomly onto a drip shield, and the model accounts for a random fraction of water that flows over the drip shield but is captured by breaches. The abstraction implemented in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Section 3.6.3.1) conservatively considered all of the seepage entering the drift as falling on the crown of the drip shield and that all fluid that drips onto the drip shield or waste package occurs at the same axial location as the breach. This analysis did not address alternative thermal operating modes, but was used to quantify conservatism in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]).

Waste Package Release Flow Geometry (Bathtub, Flow-through)–An alternative conceptual model to the flow-through geometry is the bathtub geometry, which allows seepage to collect in the waste package before being released to the Engineered Barrier System. This effect will be most important during the first 20,000 years. At longer durations (100,000 years or greater), the presence of multiple penetrations for multiple groups of waste packages makes a flow-through geometry the likely long-term configuration. This model provides estimates of the time delays for the bathtub versus the flow-through model and an approach to quantify the uncertainty and sensitivity of TSPA results to the bathtub versus the flow-through conceptual model. Alternative thermal operating modes will not affect the conceptual model for flow through the waste package.

Environment on Waste Package and Drip Shield Surfaces–Previous analyses of the possible environments on the surfaces of the waste package and drip shield focused on carbonate-based dilute waters. These waters, when concentrated by evaporation, result in high pH brines. More recent analyses have included non-carbonate based dilute waters. These are similar to the pore waters in the host rock and, when evaporatively concentrated, evolve into near-neutral pH brines with dissolved calcium and magnesium ions. The presence of these cations in aqueous solution could result in the formation of calcium and magnesium chloride salt solutions that are stable at low relative humidities. However, calcium and magnesium ions in the solution would decrease significantly during evaporation by the formation of insoluble precipitates. Thus, large quantities of seepage water would need to be evaporatively concentrated in order to form an aggressive environment. Therefore, development of calcium or magnesium chloride salt solution on the waste package and drip shield surfaces will be limited under expected repository conditions. New analyses also included assessments of the effect of potentially deleterious minor constituents, such as lead. The measured concentrations of lead in the waters at Yucca Mountain are very low. In addition, a review of data in the literature shows that sorption of lead to the surface of minerals such as smectite and calcite will limit the amount of lead in solution. Evaporative concentration of Yucca Mountain waters has shown that lead is likely removed from the solution as lead-containing mineral precipitates, and, therefore, the amount of lead available in solution is expected to be insignificant.

Aging and Phase Stability–Aging and phase stability of Alloy 22 was reevaluated using new data and analyses. These analyses confirm the prior conclusion that aging of the Alloy 22 waste package outer barrier will not pose a problem. Since this conclusion is based on limited data, alternative lines of evidence were evaluated, including mechanical property changes due to aging, natural analogues, and theoretical modeling. All of these corroborate the conclusion that for the estimated peak waste package temperatures of 200°C or lower, aging effects such as long-range ordering or grain boundary and bulk precipitation of secondary phases will not affect waste package performance.

Stress Corrosion Cracking–In the case of stress corrosion cracking of the Alloy 22 barrier, new analyses were conducted to quantify the uncertain parameters and remove conservatisms in the previous analyses. Based on new data, literature reviews, and analyses, models of the residual stress uncertainty, the threshold stress for stress corrosion cracking initiation, and the orientation of manufacturing flaws were revised. In addition, the analyses included an evaluation of the effects of temperature on stress corrosion cracking, which showed that there is currently no basis for establishing a temperature threshold for stress corrosion cracking. Some of the new data evaluated included stress corrosion cracking test data on Alloy 22 in solutions containing lead. The data show that under very aggressive (unrealistic) conditions (pH of 0.53, 250°C, and 1,300 ppm lead), Alloy 22 may fail because of stress corrosion cracking. However, tests under conditions relevant to Yucca Mountain (1 weight-percent lead in mixed-ion solutions at a pH of 2.7 and 76°C) show no stress corrosion cracking failures. Overall, the technical bases for the stress corrosion crack model were improved with the new data and analyses.

Long-Term Passive Film Stability of Alloy 22–In TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), data from relatively short-term tests (two years of exposure) were used to estimate the general corrosion rate of Alloy 22. Extrapolation of two-year data to predict performance over thousands of years was based on the assumption that the passive film on the surface would remain stable over a long period. To reduce the uncertainties associated with this assumption, a comprehensive testing and analysis program has been initiated. A mechanistic conceptual model for predicting the behavior of the passive film has been developed, and this conceptual model, along with associated model parameters, is being implemented into the passive film stability model. Preliminary calculations have been performed using values for model parameters that are based on stainless steels in nuclear power plant piping. A testing program is underway to provide data relevant to Alloy 22 for the conditions expected in the potential repository. When completed, the passive film stability model will be incorporated into the integrated waste package degradation model to analyze the effects of long-term passive film stability on waste package performance. The current model indicates that the passive film on Alloy 22 would remain stable under the exposure conditions expected in the potential repository. Data from ongoing testing programs and detailed mechanistic modeling will provide useful information to determine the long-term stability of the passive film under repository-relevant exposure conditions.

General Corrosion of Alloy 22–Previous analyses of Alloy 22 general corrosion were based on data from weight-loss measurements on samples exposed for approximately two years. Because of the low corrosion rates in the material, the data showed significant uncertainties that are due mostly to measurement uncertainty. As a result, the data showed no discernible effects of temperature, environment, or exposure times on corrosion rates. New analyses based on new electrochemical data have been conducted to evaluate the effects of temperature on the Alloy 22 general corrosion rate. While the correlation developed is based on limited data over a small temperature range, the model provides a basis for evaluating waste package performance over ranges of time and location in the potential repository. The updated model indicates that inclusion of temperature dependence in the process models for waste package degradation will result in decreased corrosion rates, and longer waste package lifetimes, than previous analyses. The increased lifetimes are reflected in the performance analyses described in Volume 2 (McNeish 2001 [DIRS 155023]).

Early Waste Package Failure: Improper Heat Treatment–For the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) model, an extensive literature review was conducted to identify scenarios or conditions that could lead to early failure of waste packages. Mechanisms that could lead to early failure, except for weld flaws in the closure weld area, were considered but not included in the TSPA-SR model. This exclusion was based on the low probability of the individual mechanisms and the planned use of administrative controls to further reduce the likelihood of early failure mechanisms. In reevaluating the potential for early failure mechanisms and their potential consequences for the SSPA, a more conservative approach was adopted. This approach resulted in the inclusion of an improper heat treatment event which conservatively results in the subsequent failure of the waste packages in the supplemental total system performance analyses described in Volume 2 (McNeish 2001 [DIRS 155023]). This non-mechanistic model results in the early failure of a small fraction of the waste packages. To ensure that the potential consequence of early waste package failures is treated conservatively, it is included in the nominal scenario for the performance assessment, not as a sensitivity analysis. The analysis results show that the probability of having at least one waste package improperly heat-treated in the potential repository is 20.2 percent, and the probability of having two waste packages affected is 2.6 percent. Assuming a total of 100 realizations for the waste package degradation analysis model, those probabilities provide that about 77 out of 100 realizations would have no waste packages affected by improper heat treatment. Out of 100 realizations, about 23 realizations would have at least one waste package affected.

15.3 KEY ATTRIBUTE: LIMITED RELEASE OF RADIONUCLIDES FROM THE ENGINEERED BARRIERS

The processes that influence the potential dissolution and transport of radionuclides that could occur after a waste package is breached are described in Sections 9 and 10 of the SSPA. As described in the S&ER (DOE 2001 [DIRS 153849]), the key processes affecting performance include the degradation of spent fuel cladding, and commercial and DOE high-level radioactive waste glass, which depend on the chemical environment inside the waste package. After the spent fuel or high-level radioactive waste glass is degraded, the processes controlling repository performance include the dissolution or colloid associated suspension of radionuclides, and the potential transport of radionuclides through the package and the engineered barrier system.

In the SSPA, analyses of uncertainties in transport processes within the Engineered Barrier System were performed to provide insight into the uncertainties recognized in the S&ER (DOE 2001 [DIRS 153849]). In general, these analyses indicate that uncertainty in the relevant processes either did not significantly affect performance (e.g., high-level radioactive waste glass dissolution rates, cladding degradation) or that the assumptions used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) were conservative (e.g., radionuclide solubilities). In addition, several improved process model representations (e.g., neptunium solubility, diffusion inside the waste package) were developed and implemented in the TSPA described in Volume 2 (McNeish 2001 [DIRS 155023]). These updated models replaced conservative representations in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), generally resulting in delays in releases of radionuclides from the Engineered Barrier System.

Lower-temperature operating modes do not have a significant effect on glass degradation rates, radionuclide solubilities, diffusion or other transport processes within the engineered barriers. These processes only occur after waste packages are breached, which is generally at a time when the thermal differences between operating modes are negligible.

Effect of High-Level Waste Glass and Steel Degradation Rate on In-Package Chemistry– The effect of uncertainties in high-level waste and steel degradation rates on in-package chemistry was evaluated in a series of sensitivity studies wherein a wide range of waste form component degradation rates were used as input into reaction-path calculations. This allowed better quantification of the limits of fluid compositions likely to prevail in breached waste packages. Changing the input reaction rates has the effect of altering the assumed proportion of waste form components with which incoming fluids might react. Consequently, this approach allows an assessment of the effects of heterogeneous inflow contact with waste form materials on in-package chemistry and the effect of uncertainties in the input degradation rates on in-package chemistry. Reaction-path outputs suggest only minor deviations from earlier predictions of in-package chemistry bounds. One exception is the case of zero dissolution of A516 steel wherein the minimum in-package pH tends to drop down to between pH 2 and 3, which increases the abstracted uncertainty range.

Effect of Creep Rupture, Localized Corrosion, Seismic Failure, Rock Overburden Failure, and Unzipping Velocity on Cladding Degradation–An improved irradiated cladding creep correlation and failure criteria were developed. The localized corrosion model was improved to include corrosion in damp waste packages (no dripping) and a less conservative cumulative complementary distribution function. A sensitivity study showed little effect from a more precise seismic frequency curve for cladding damage. The effect of cladding failure from a rock overburden after waste package degradation has been added.

U.S. Department of Energy High-Level Radioactive Waste Degradation Rates–The effect of variable DOE high-level radioactive waste degradation on in-package chemistry was assessed in a series of reaction-path calculations that used as input a spectrum of different DOE high-level radioactive waste degradation rates. Degradation of DOE high-level radioactive waste might occur at different rates due, for example, to the buildup of reaction-limiting secondary mineral phases at the glass-solution interface. Calculations indicated that DOE high-level radioactive waste rates lower than the values presently used result in a pH range in the in-package fluids that is substantially less alkaline. This pH-lowering works against radionuclide transport in some cases (i.e., when pH is lowered from 10 to 9), but more favorable in others (e.g., if pH is lowered from 4 to 3). The latter scenario has been used to expand the abstracted uncertainty range in in-package pH. New, more detailed abstractions of pH-time trajectories were developed for commercial spent nuclear fuel and codisposal waste forms.

Solubility of Neptunium, Thorium, Uranium, Plutonium, and Technetium–The solubilities of thorium, plutonium, and technetium were more closely examined using a much wider variety of in-package scenarios than the conservative bounding case considered in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). The latter assumed uniformly oxidizing conditions and that amorphous, hydrated oxide minerals controlled the dissolved levels of thorium and plutonium as opposed to the more crystalline phases that might form over longer periods of time. Pooling of water and degradation of metallic in-package components might cause lower oxygen fugacities to prevail, thus stabilizing reduced forms of plutonium and technetium. Moreover, long periods of reaction might favor the conversion of soluble oxide minerals to thermodynamically stable, but less soluble, oxides. Sensitivity tests showed that the presence of less soluble oxides and lower oxygen fugacities lead to predictions of much lower dissolved concentrations of thorium, plutonium, and technetium.

A new model of neptunium release from fuel was calibrated using solid solution analysis and neptunium concentrations derived from ongoing fuel degradation tests at Argonne National Laboratory and Pacific Northwest National Laboratory.

Colloid Mass Concentrations–Unquantified uncertainties in the waste form colloid model were examined to more closely model colloidal uptake of radionuclides. The number of corrosion product colloids were combined with the groundwater colloid abundance and their sum assigned an uncertainty distribution. The mean value was based on deep groundwater analyses. A log normal distribution of radionuclide sorption K_ds was then developed. A probability distribution was likewise developed to describe irreversible sorption of plutonium on waste form colloids.

Diffusion Inside Waste Package–The current TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) transport model for the waste package conservatively assumes that all radionuclides released by the waste form are immediately available to diffuse through any breaches in the package. This approach is equivalent to assuming instantaneous in-package diffusion. A new model for diffusion inside the waste package was developed that incorporates information on the adsorption of water vapor on iron-(hydr)oxides, on Zircaloy oxides, and on nickel oxide, which are anticipated to exist in the waste package once corrosive processes begin after the package is breached. The model calculates diffusion rates through the films of water adsorbed onto corrosion products. The general approach for commercial spent nuclear fuel waste packages is to consider three limiting pathways for diffusion: along failed fuel rods, through porous corrosion products inside the package, and through porous corrosion products filling breaches (either stress corrosion cracks or general corrosion patches) in the outer layer of the waste package. The diffusive flux for releases along failed fuel rods and through corrosion products within the package is calculated, and the larger of these two is selected (radionuclides will diffuse along the fastest independent pathway that is available). Next, the diffusion rate through breaches in the package is computed. The smaller of the in-package diffusion rate and the breach diffusion rate is selected as the net diffusive release. This is reasonable because these pathways are sequential so the smallest diffusion rate will be the controlling parameter.

The model quantifies the impact of in-package diffusion on radionuclide transport for commercial spent nuclear fuel waste packages in a non-dripping environment.

Transport Pathway From Inside Waste Package to Invert–A detailed advective-diffusive transport model between the waste form and the invert has not been incorporated in performance assessment analyses. This approach is reasonable because three-dimensional predictions of relative humidity and waste package temperature are not currently available to the required level of detail, the effects of surface roughness and heterogeneity may be significant but have not been studied in detail, and there is a wide range in the maximum value of relative humidity that will prevent advective transport. Additional research on thin film flow is ongoing, and sensitivity results will be evaluated to determine the impacts from the other models introduced in this section.

Sorption Inside the Waste Package–Two approaches have been used to estimate ranges of partition coefficients in the engineered barrier system. The first approach utilizes median values and ranges for partition coefficients (K_ds) for americium, iodine, neptunium, plutonium, technetium, thorium, and uranium on typical soils and corrosion products, or under oxidizing conditions from a variety of sources. The second approach to estimating the appropriate ranges of values for partition coefficients is based on the concept of tolerance interval. Tolerance intervals provide a statistical estimate of parameter ranges at a given confidence level from a small data set. The final recommendations for partition coefficients and distribution type are based on a merging of these two approaches. At the low end, each range is based on the minimum value from the tolerance interval because it provides a 95 percent level of confidence using data for sand, loam and clays. At the high end, each range is based on the maximum value for the corrosion products because the tolerance interval often has values that appear unusually high.

Sorption Inside the Invert–The approach for sorption inside the invert is identical to that for sorption inside the waste package, as discussed above.

Diffusion Through the Invert–The diffusion coefficient abstraction for the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) includes the effects of invert porosity, invert saturation, invert temperature, and the uncertainty in the experimental measurements for the diffusivity of granular materials. Analyses were conducted to evaluate conservatism in the dependence of diffusivity on porosity, to quantify conservatism in using the self-diffusivity of water as a bounding value for all radionuclides of interest for TSPA, and to evaluate uncertainty in using a volume averaged saturation for the invert versus a more detailed saturation gradient for diffusive transport. The formulation for the dependence of diffusivity on porosity for the TSPA-SR sensitivity studies reduces the diffusion coefficient by 32 percent in comparison to the value used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) at a porosity of 50 percent. The conservatism in using the self-diffusivity of water as a bounding value for the diffusion coefficient is a factor of 1.07 to 3.8, and is a function of the valence of the species. The uncertainty in using the volume-averaged saturation for the invert is very small because the invert saturation state beneath the waste package is almost uniform from the top of the invert to the bottom of the drift.

Colloid Stability in the Invert–The goal of this analysis is to quantify the impacts of uncertainties in the behavior of colloids generated from the degradation of high-level radioactive waste glass, commercial spent nuclear fuel, and DOE spent nuclear fuel, as well as colloid-facilitated transport properties of radionuclides in the engineered barrier system. The current TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) model for generation and transport properties of colloids resulting from waste form degradation generally uses a bounding approach for incorporating relevant source data, and it uses conservative assumptions where the available data were thought to be limited. Uncertainties have been quantified for the combined concentrations of groundwater and corrosion colloids, for plutonium irreversibly attached to waste form colloids, and for the reversible sorption of plutonium and americium on waste form and groundwater colloids. The uncertainties in the combined concentrations of groundwater and corrosion colloids have been characterized for a low and a high range of ionic strength. Distributions for plutonium irreversibly associated with waste form colloids were selected to capture the potential uncertainty for and sensitivity to irreversible plutonium sorption in the present study, in a way that tests the entire ranges of values uniformly. Finally, a preliminary review suggested that the currently used K_d values for iron-(hydr)oxides (proxy colloid mineral for steel corrosion colloids) may be underestimated by as much as one to two orders of magnitude. Considering the large mass of iron-(hydr)oxides that may be present in the engineered barrier, it is reasonable to use the same distribution for K_ds that describe the sorption of plutonium and americium onto colloids. The recommended distribution for this study is a log normal distribution with a mean value of 10^5 mg/L and a standard deviation of two orders of magnitude.

Microbial Transport of Colloids–The goal of this model is to quantify the impact of potential microbial communities on sorption of radionuclides to microbes and the ability of microbes to be transported as colloids through the engineered barrier system. The transport of microbes through the engineered barrier system is a function of the uptake of dissolved radionuclides onto the cell walls and the subsequent mobility of microbes through the waste package and invert. The representation of uncertainty for the microbial transport model is based on the distribution for uptake of uranium and plutonium on microbes. The uptake of uranium for sensitivity studies will be a triangular distribution with a range between 45.2 and 615 mg uranium/gm and with a median value of 111.33 mg uranium/gm. Plutonium and thorium are also expected to sorb onto microbes. Because there are no specific data for uptake of these two elements, the sampled value from the distribution for uranium uptake will be scaled to the relative abundances of plutonium and thorium versus that of uranium.

15.4 KEY ATTRIBUTE: DELAY AND DILUTION OF RADIONUCLIDE CONCENTRATIONS BY THE NATURAL BARRIERS

Sections 11 (Unsaturated Zone Radionuclide Transport), 12 (Saturated Zone Radionuclide Transport) and 13 (Biosphere) of the SSPA describe the processes that contribute to delaying and reducing the concentrations of any radionuclides that may be released from the potential repository. Important transport processes acting in the natural barriers beneath Yucca Mountain include the effects of a drift shadow (a zone of reduced water saturation below emplacement drifts) in the unsaturated zone, and matrix diffusion and sorption in both the unsaturated and saturated zones.

In the SSPA, a series of evaluations was performed to assess the sensitivity of flow and transport calculations to uncertainties in flow processes, and to variability and uncertainty in hydrologic properties in volcanic rocks and alluvium. Improved models were developed that describe the colloidal transport of radionuclides, and the potential for sorption of radionuclides in alluvium. In most cases, the uncertainty analyses and the improved models indicate that the simplified models used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) are conservative, and that the unsaturated and saturated zones are likely to delay and reduce radionuclide concentrations more than previous analyses indicated. In one case (sorption coefficient for iodine and technetium in alluvium), the parameter values used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) were judged to be non-conservative based on recent information, so the saturated zone transport model was revised accordingly.

Analysis of the possible effects of LTOMs on radionuclides transport away from the potential repository indicates that thermal effects on transport properties and processes are likely to be small and not significantly affect performance.

Effect of Drift Shadow Zone–The hydrologic conditions beneath waste emplacement drifts are affected by the diversion of seepage around the drift. This diversion of seepage results in a zone of reduced water saturations and flow beneath waste emplacement drifts. An important aspect of radionuclide transport near the drift is how radionuclides enter the rock. Radionuclides can enter the rock from waste emplacement drifts as a result of diffusive transport or a combination of advection and diffusion. If seepage into the drift is substantial, the radionuclides will be advected out of the drift predominantly into the rock fractures. If seepage into the drift is sufficiently small, radionuclides will either advect or diffuse predominantly into the rock matrix. Diffusive releases of radionuclides from the drift will predominantly enter the rock matrix because its water content is considerably larger than the water content of the fractures, providing a greater cross section for diffusion. Initiating transport in the rock matrix, rather than the fractures, can substantially reduce the rate of radionuclide movement away from the drift. This is primarily caused by the limited contact between the fractures and the matrix, which is consistent with calibration of the unsaturated zone flow model and geochemical observations. The result is long residence times in the slow-flowing matrix. Furthermore, the reduction in water saturation in the fractures beneath the drift enhances the retention of radionuclides in the matrix. An approximate representation of the drift shadow is included in TSPA by defining the release domain according to the Engineered Barrier System-to-rock transport mechanism. Diffusive releases from the Engineered Barrier System enter the rock matrix and advective releases enter the rock fractures. Other aspects of the drift shadow, in particular the reduced saturations and flow velocities in this zone, are not included in the present TSPA implementation.

Matrix Block Discretization Effects–Dual-permeability models of unsaturated zone radionuclide transport in fractured rock commonly use a single matrix gridblock associated with each fracture gridblock. The single-matrix-grid model must approximate radionuclide concentration gradients leading to diffusion between the fractures and matrix in terms of a single matrix concentration. In reality, a continuous range of concentrations in the matrix will result from radionuclide concentration differences between the fractures and matrix. This continuous range of concentrations can be more accurately captured using multiple-matrix gridblocks associated with each fracture grid. A comparison of transport calculations using a single-matrix grid model and a multiple-matrix grid model shows that the leading edge of a radionuclide breakthrough curve will arrive significantly earlier using the single-matrix grid model. Transport at later times in the breakthrough are not appreciably affected by the single-matrix grid approximation. Thus, the results indicate that a single-matrix grid model is a conservative predictor for radionuclide transport behavior. More refined approaches to evaluating radionuclide transport include multiple-matrix gridblock models for flow and transport, for transport but not for flow, and alternative calculation schemes such as particle tracking methods.

Calculation Methods for Radionuclide Transport–Calculation schemes for radionuclide transport include particle-tracking methods and direct numerical solution of the conservation equations. The different schemes can result in different model predictions, particularly due to the differences in the approaches used for matrix diffusion. Simulation results from three different simulation methods for unsaturated zone transport are described. All three methods use the same dual-permeability grid, consisting of overlapped meshes that represent fracture and matrix continua. Although the three simulation methods tested agree for certain problems, differences between the particle-tracking method used for TSPA-SR and the process-level models were found for transport calculations involving dual-permeability systems. These differences are attributable to simplifying assumptions used in the TSPA-SR particle-tracking algorithm that provide a more efficient calculation scheme for capturing concentration gradients in the matrix. Improvements in an alternative particle tracking method is found to also provide a more accurate representation of matrix concentration gradients for fracture-matrix diffusive exchange than the baseline version, while avoiding some of the assumptions used in the TSPA-SR algorithm.

Effects of Potential Repository Footprint on Three-Dimensional Transport–Radionuclide transport in the unsaturated zone between the potential repository and the water table is dependent on the location, size, and shape of the potential repository (i.e., the repository footprint). This results from the unpredictable location-specific geologic and hydrologic variability present in a natural system. Sensitivity calculations were performed to investigate the changes in radionuclide-transport behavior from the potential repository to the water table if the baseline potential repository footprint should be extended to the south. The results of the investigation found that radionuclide transport in the extended footprint were slower than in the baseline potential repository block, although the differences were not large (e.g., mean breakthrough times differ by less than a factor of 2). Uncertainties with regard to footprint effects on radionuclide transport are primarily caused by uncertainties in the footprint itself (i.e., the potential repository design) and in the geologic characterization for regions that lie outside the baseline footprint. This uncertainty is treated by using a range of flow models.

Effects of Thermally-Driven Coupled Processes–Thermal energy from the potential repository will induce thermal-hydrologic and thermal-hydrologic-mechanical couplings that affect flow, and thermal-hydrologic-chemical couplings that affect flow as well as geochemical conditions. All of these processes affect the conditions for radionuclide transport. Because the heat source is located in the waste emplacement drifts, the effects of these coupled processes tend to be more pronounced near the waste emplacement drifts. The thermal-hydrologic flow coupling is primarily caused by vaporization/condensation phenomena that result in redistribution of water and changes in flow patterns. The thermal-hydrologic-mechanical coupling affects flow behavior through changes in hydrologic characteristics resulting from induced mechanical strain in the rock. The thermal-hydrologic-chemical coupling can cause changes to hydrologic properties through precipitation/dissolution of minerals, as well as aqueous and mineralogical changes that can affect radionuclide sorption and colloid behavior. Process-model evaluations concerning thermal-hydrologic effects on mountain-scale flow indicated that effects on radionuclide transport should be minimal. However, the dryout near the waste emplacement drift may result in significant delays in radionuclide transport for the high-temperature case. The effects of thermal-hydrologic-mechanical coupled processes on radionuclide transport were found to cause only relatively small changes in hydrologic properties; hence the effects on flow and transport should be minimal. Similarly, thermal-hydrologic-chemical coupled processes were found to cause only relatively small changes in hydrologic properties and, therefore, should not have much effect on radionuclide transport.

Groundwater Specific Discharge Uncertainty–In the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), specific discharge in the site-scale saturated zone flow and transport model is represented as three discrete cases: high, medium, and low. The value for the low case was one-tenth of the value for the medium case, and the value for the high case was 10 times that of the medium case (0.6 m/yr). In sensitivity studies performed as part of the saturated zone unquantified uncertainty analysis, the range of specific discharge was reduced such that the low- and high-value cases were one-third and three times the medium value, respectively.

Effective Diffusion Coefficient in Volcanic Tuffs–The probability distribution for radionuclide effective diffusion coefficients was modified from log uniform to log-triangular probability distribution. The upper and lower bounds are still the same as in TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), 10^{-10} and 10^{-13} m²/s, respectively, but the most probable value is 3.2×10^{-11} m²/s. The basis for this was to put more emphasis on the mean value compared to sampling a uniform distribution that results in sampling equally all values in the distribution.

The effect of this change is that larger and smaller effective diffusion coefficients are less probable.

Flowing Interval (Fracture) Porosity, Enhanced Matrix Diffusion Case–The probability distribution for flowing interval porosity was modified from a log-uniform to a log-triangular distribution with a lower bound of –5.0, a most-likely value of –3.0, and an upper bound of –1.0 (the same upper and lower bounds as the TSPA-SR). This distribution places more weight at the mid-point of the distribution range compared to the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) uniform distribution, which results in equal probabilities for the given range.

Effective Porosity in the Alluvium–The probability distribution used for effective porosity in the alluvium was modified to a probability distribution that is more representative of preliminary results from single-well, isolated-interval hydraulic tests at well NC-EWDP-19D1. The distribution used for the SSPA Volume 2 (McNeish 2001 [DIRS 155023]) calculation was changed from a truncated normal distribution with a mean of 0.18, a standard deviation of 0.051, a lower bound of 0, and an upper bound of 0.35, to a normal distribution with a mean of 0.15, a standard deviation of 0.051, a lower bound of 0, and an upper bound of 0.30.

Correlation of the Effective Diffusion Coefficient with Matrix Porosity–Sampled matrix diffusion coefficients were correlated with matrix porosities using a relationship developed from laboratory diffusion-cell experiments. These experiments measured anion diffusion coefficients through tuff matrices from various stratigraphic units from the C-wells Complex and from Pahute Mesa at the Nevada Test Site.

Bulk Density of the Alluvium–New average dry bulk density values were estimated based on a saturated bulk density and porosity measurements from a borehole gravimetry survey in well NC-EWDP-19D1. Based on the new data this parameter was represented stochastically for the unquantified uncertainty analysis. The value for dry bulk density in the alluvium is changed from a constant value of 1.27 g/cm^3 to a stochastic variable that is more representative of uncertainty for dry bulk density at Yucca Mountain. The new dry stochastic bulk density is based on data from well NC-EWDP-19D1 and is represented by a normal distribution with a mean of, 1.91 g/cm^3, and standard deviation, 0.080 g/cm^3.

Retardation for Radionuclides Irreversibly Sorbed on Colloids in the Alluvium–Alluvium grain size distributions from well NC-EWDP-19P and from other locations at the Nevada Test Site were used to refine estimates of colloid filtration rate constants in the alluvium. This well was drilled using an air-hammer method that preserved smaller and larger grain sizes much better than rotary drilling methods. The revised cumulative distribution function for the retardation factor of radionuclides that are irreversibly sorbed to colloids in the alluvium was generated using the same equations and procedure as the cumulative distribution function in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]).

Presence or Absence of Alluvium–This sensitivity analysis is bounding in the sense that flow path length in the alluvium is reduced to the minimum reasonable value, based on current geologic data. However, it is not absolutely bounding because it still includes approximately 1 to 2 km of alluvium at the end of the flow path near the 20-km point of compliance.

The minimum-alluvium sensitivity analysis is implemented in the site-scale saturated zone flow and transport model by reducing the extent of the alluvium uncertainty zone to zero.

Sorption Coefficient in Alluvium for Iodine and Technetium–Further analysis of batch sorption data of technetium-99 and iodine-129 (as TcO_4^- and I^-) onto alluvium samples, as well as recent technetium-99 and iodine-129 column test results, indicate that sorption distribution (K_d) values for technetium-99 and iodine-129 sorbing onto the alluvium are zero under oxidizing (ambient) conditions. Therefore, sorption coefficients in the alluvium for iodine and technetium were considered to be zero in the saturated zone transport model.

Sorption Coefficient in Alluvium for Neptunium and Uranium–New results from two column experiments for K_d values for neptunium-237 in the alluvium have been performed in which the effective K_d values of neptunium-237 were significantly lower than values measured in batch sorption experiments with the same material used to pack the columns. Therefore, the probability distribution for neptunium sorption coefficient in the alluvium was changed from a probability distribution based on laboratory batch experiments to one that represents batch and column laboratory experiments. The distribution function gives considerable weight to the column experiments, which weights the lower sorption-coefficient values. Based on the absence of experimental data on uranium sorption coefficients in alluvium, the probability distribution for uranium is represented as the sorption-coefficient probability distribution for neptunium in the alluvium.

Sorption Coefficient for Neptunium in Volcanic Tuffs–The probability distribution used for the neptunium sorption coefficient in the matrix was changed from a probability distribution based on a vitric rock type to a probability distribution that is more representative of the rock types that the flow path will encounter. For a given set of realizations (i.e., simulations with Monte Carlo sampling) the new probability distribution is determined by sampling the vitric distribution approximately 67 percent of the time and the zeolitic distribution 33 percent of the time.

K_c (Reversible Colloids) Model for Groundwater Colloid Concentrations–The sensitivity analysis for the saturated zone consists of simulation of radionuclide breakthrough curves for the two classes of radionuclides associated with the reversible colloid model: strongly sorbing radionuclides (plutonium, americium, and thorium) and moderately sorbing radionuclides (strontium, cesium, and protactinium). These simulations are implemented in the site-scale saturated zone flow and transport model using resampled values for the K_c parameter and for the K_d of strongly sorbing radionuclides. The values for the K_c parameter used in this analysis are based on sampling of uncertainty distributions for the K_d of americium onto colloids and for the concentration of colloids in the groundwater, as explained in Volume 2 (McNeish 2001 [DIRS 155023], Section 3). The uncertainty distribution for K_d of strongly sorbing radionuclides onto the alluvium material is changed to beta distribution with greater statistical mass near the expected value of 50 ml/g (McNeish 2001 [DIRS 155023], Section 3). Other stochastic parameters for the saturated zone have the same values for the sensitivity analysis as the SSPA Volume 2 (McNeish 2001 [DIRS 155023]) supplemental analysis.

Enhanced Matrix Diffusion–For this case, most of the rock matrix in the volcanic units is available for radionuclide storage and sorption in the transport process in most of the realizations. The sensitivity analysis for the enhanced-matrix-diffusion case is implemented by reducing the flowing interval spacing by two orders of magnitude for all realizations. This approach reduces the geometric mean of the flowing interval spacing from about 20 to 0.2 m, which is a relatively small distance for matrix diffusion. Other stochastic parameters for the saturated zone have the same values for the sensitivity analysis as the SSPA Volume 2 (McNeish 2001 [DIRS 155023]) supplemental analysis.

No Matrix Diffusion–The sensitivity analysis for no matrix diffusion is implemented in the site-scale saturated zone flow and transport model by reducing the value of the effective matrix diffusion coefficient by ten orders of magnitude in all realizations. This large reduction in the matrix diffusion coefficient effectively renders the simulated radionuclide mass delay to matrix diffusion insignificant. Other stochastic parameters for the saturated zone have the same values for the sensitivity analysis as the SSPA Volume 2 (McNeish 2001 [DIRS 155023]) supplemental analysis.

Biosphere Uncertainty Analyses for Groundwater and Igneous Releases–Because of the location of the receptor, the reference biosphere is sufficiently distant from the engineered barriers component of the potential repository that there are no direct interactions between these two system components. Thus, the thermal operating conditions within the repository have no effect on the reference biosphere or the dose predictions. Therefore, the new biosphere analyses only address the effect of new data and of previously unquantified uncertainties. Biosphere dose conversion factors (BDCFs) were developed based on revised input for all the radionuclides in TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) plus selenium-79 and neptunium-237. These BDCF data were generated for the radionuclides released into the biosphere with contaminated groundwater and contaminated volcanic ash. The robustness of the biosphere approach was investigated by performing sensitivity studies on the impact on both BDCFs and annual dose of the definition of the human receptor and alternative dose assessment methodologies as recommended by the International Commission on Radiological Protection. The uncertainties in BDCFs for important radionuclides were quantified for several parameters that had previously been considered fixed and not subject to uncertainty. Examples of such uncertainties are leaching factors, weathering factor for removal of contamination from plant leaves, and translocation factors. In addition, the change in BDCF values and annual groundwater usage due to projected climate change was assessed.

15.5 KEY ATTRIBUTE: LOW MEAN ANNUAL DOSE CONSIDERING POTENTIALLY DISRUPTIVE EVENTS

Section 14 of the SSPA describes analyses completed to incorporate new information about the potential for disruptive events at Yucca Mountain, and to assess the effect of LTOMs on the probability that disruptive events could affect the performance of a potential repository. The possible changes in the footprint of the repository associated with alternative operating modes could slightly change probability calculations that depend on the spatial extent of the repository.

In addition to the analyses related to the configuration of the repository, the DOE has developed improved models that describe the possible consequences of volcanic eruptions. In general, the changes to the probability estimates and the process models for disruptive events at Yucca Mountain are small and do not significantly affect repository performance.

Probability of Dike Intrusion–Additional analyses have been conducted to evaluate the probability distribution for dike intrusion for the repository footprint described in the S&ER (DOE 2001 [DIRS 153849]). The evaluations were carried out for operating modes both with and without backfill. The effort characterized the probability distribution for the annual frequency of dike intersection with the potential repository footprint for the primary block and for the primary and contingency block combined. Other distributions required to evaluate the consequences of the event were derived. These parameters include the length and orientation of the dike intersection with respect to the repository and the number of conduits (or eruptive centers) with the footprint of the potential repository.

Scaling Factors to Evaluate Impacts of Alternative Operating Modes–The degree of interaction between a dike and the waste entombed in the potential repository is dependent upon the configuration of the facility. The degree of interaction is dictated by such factors as footprint area, footprint location, drift spacing, and waste package spacing. This effort derived scaling factors to allow an approximate but rapid evaluation of the effect that alternative operating modes and repository configurations could have on the probability and consequences of volcanic events.

Calculation of Contribution of Releases from Zones 1 and 2–In the igneous intrusion scenario, damage to waste packages in drifts intersected by an igneous dike is divided into two zones. In Zone 1, damage is extensive and the waste package provides no further protection to the waste. In Zone 2, waste packages are also damaged, but still provide some protection. In the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), Zones 1 and 2 were treated jointly. For the uncertainty study, the relative contributions to dose from Zone 1 and Zone 2 were determined. Results are reported in SSPA Volume 2 (McNeish 2001 [DIRS 155023]). Because backfill would minimize magma transport along any intersected drift, Zone 2 phenomenology only applies to the non-backfill case. This study allowed a more complete understanding of the total system performance assessment results for the intrusive groundwater release scenario.

Sensitivity to Waste Particle Size Distribution–Particle size distribution of the ash from a volcanic event plays a dominant role in determining the characteristic of the atmospheric transport of the ash. The waste particle size distribution and their interaction with the ash particles during the event play a potentially significant role in determining the dose consequence of that event. The volcanic predictive capability (ASHPLUME V1.4LV-dll) that is run in TSPA-SR was provided with a set of reasonable particle (ash and waste) size distribution to enable a sensitivity study to be conducted. The results of this study are presented and discussed in Volume 2 (McNeish 2001 [DIRS 155023]).

New Wind Speed Data for Various Heights of Eruption–The transport of ash during an eruption, with any entrained contaminants, is a function of many factors such as eruption characteristics and atmospheric conditions. In TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) a simple atmospheric model was used that assumed the wind velocity (speed and direction) was a constant and independent of altitude. The wind speed cumulative distribution function was based on data gathered at altitudes of approximately 1,500 to 5,000 m above sea level. Because of the potential for an eruptive plume of ash to extend higher than 5,000 m into the atmosphere, a new cumulative distribution function for wind speed was developed based on an alternative data set. These data were acquired from an average height of 9,434 m and are consistent with possible plume heights for the Yucca Mountain region. The maximum and median of the new distribution function are approximately twice those used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) and form the basis for a sensitivity analysis in SSPA Volume 2 (McNeish 2001 [DIRS 155023]).

Method for Handling Ash/Waste Particle Density–Ash particle density is an important parameter in the code used to model the dispersion of waste-contaminated volcanic ash in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). Density affects the calculation of the terminal velocity of a particle as it settles in the atmosphere. In the code, ash particle density is appropriately modified when an ash particle is combined with a waste particle.

Volcanism Inputs for Supplemental TSPA Model–Updated information consistent with the current understanding of the probability and consequences of disruptive events has been incorporated in the analyses described in Volume 2 (McNeish 2001 [DIRS 155023]).

Potential Impact of New Aeromagnetic Data on Probability of Dike Intrusion–The U.S. Geological Survey has gathered new aeromagnetic data for the Amargosa Valley/Crater Flat/Yucca Mountain region. These data are being assessed to evaluate the likelihood that magnetic anomalies identified in the survey represent buried volcanoes and, if so, provide information on their properties. These results will then be evaluated to determine whether additional steps are needed. It is probable that the presence of any newly identified igneous features would not significantly impact performance assessment results because they would be accounted for by the uncertainties already included in the model. However, assessing the impact of the new aeromagnetic survey data will depend on the outcome of a full analysis of these data.

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APPENDIX A
HUMAN INTRUSION SCENARIO

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HUMAN INTRUSION SCENARIO

Introduction–The EPA standard in 40 CFR 197.25 (66 FR 32074 [DIRS 155216]) requires that the DOE determine when a human intrusion could occur based upon the earliest time that current technology and practices could lead to waste package penetration without the driller noticing. The EPA standard also establishes different dose standards, based on the earliest time (i.e. at or before 10,000 years after disposal or occurs more than 10,000 years after disposal) that a complete waste package penetration is projected to occur unnoticed. The proposed NRC rule states that, rather than speculating on the nature and probability of future intrusion, it is more useful to assess how resilient the geologic repository would be against a postulated intrusion (64 FR 8640 [DIRS 101680], p. 8675) and requires an assessment of repository performance based on a postulated human intrusion occurring 100 years after permanent closure. The DOE included in proposed 10 CFR 963.16 (64 FR 67054 [DIRS 124754]) the requirement for a performance assessment of stylized human intrusion into the repository as defined by NRC regulations (64 FR 67054 [DIRS 124754], p. 67079). The stylized human intrusion scenario takes the form of a drilling event that results in a single, nearly vertical borehole that penetrates a waste package, extends to the saturated zone, and is not adequately sealed (64 FR 8640 [DIRS 101680], p. 8677). To evaluate the likelihood of compliance with these requirements, the DOE evaluated two stylized human intrusion scenarios in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). Figure 4.4-12 of the TSPA-SR shows a comparison of the mean human intrusion annualized dose curve from an intrusion at 100 and 10,000 years.

The purpose of this appendix is to provide a preliminary analysis of whether a driller would likely notice, based on current technology and practices, the complete penetration of a waste package at or before 10,000 years or more than 10,000 years after disposal.

Regulatory Basis–The EPA standard published in 40 CFR 197.25 (66 FR 32074 [DIRS 155216]) requires that the DOE determine when a human intrusion could occur based upon the earliest time that current technology and practices could lead to waste package penetration without the drillers noticing that the waste package had been penetrated.

Proposed NRC rule 10 CFR 63 (64 FR 8640 [DIRS 101680]) includes requirements that the DOE potential repository design must still perform as intended if an assumed, stylized intrusion occurs (64 FR 8640 [DIRS 101680], p. 8651). The NRC has proposed that DOE use current practices for resource exploration to establish properties (e.g., diameter of the borehole, drilling rate, composition of drilling fluids) for the intrusion scenario. The proposed rule requires an assessment of the ability of the geologic repository to limit radiological exposures in the event of limited human intrusion into the engineered barrier system. Compliance is to be demonstrated through a separate performance assessment that meets the requirements specified at proposed 10 CFR 63.114 (64 FR 8640 [DIRS 101680]) and uses the reference biosphere and critical group specified at proposed 10 CFR 63.115 (64 FR 8640 [DIRS 101680]). The assessment has to assume that the human intrusion occurs 100 years after permanent closure and takes the form of a drilling event that results in a single, nearly vertical borehole that penetrates a waste package, extends to the saturated zone, and is not adequately sealed. (64 FR 8640 [DIRS 101680], p. 8677).

The DOE has also included, in proposed 10 CFR 963.16 (64 FR 67054 [DIRS 124754]), a requirement to determine postclosure suitability based on TSPA analyses of repository performance in cases with and without a stylized human intrusion event (64 FR 67054 [DIRS 124754], p. 67073). The requirements for this second TSPA include the assumptions for a stylized human intrusion into the repository, as defined by NRC regulations (64 FR 67054 [DIRS 124754], p. 67079).

Performance Assessment Background–The considerations used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246] Section 4.4) for a stylized human intrusion into the repository are summarized in Table 4.4-1 of the TSPA-SR. The stylized human intrusion was assumed to occur 100 years following permanent closure. TSPA-SR Figure 4.4-11 shows 300 simulated annualized dose histories along with some statistical measures of the annualized dose distribution. The peak mean human intrusion annualized dose during the first 10,000 years after potential repository closure is approximately 0.008 mrem/yr., occurring at approximately 1,000 years. No annualized dose for any of the 300 realizations exceeds 0.5 mrem/yr over the first 10,000 years. TSPA-SR Figure 4.4-12 shows a comparison of the mean human intrusion annualized dose curve from an intrusion at 10,000 years with the mean annualized dose curve from the base case intrusion at 100 years. For the intrusion at 10,000 years, there were no annualized doses prior to 10,000 years and the peak mean annualized dose over 100,000 years is less than that for the base case intrusion at 100 years. At 100,000 years, the mean annualized dose is nearly identical to the mean annualized dose from the base case, and is approximately 0.004 mrem/yr. (CRWMS M&O 2000 [DIRS 153246], Section 4.4)

The results of the TSPA-SR drip shield and waste package studies indicate long lifetimes for these components (CRWMS M&O 2000 [DIRS 153246], Section 3.4), with the first drip shield failures occurring after about 20,000 years. The first failures of the waste package outer material, Alloy 22, by general corrosion occur after approximately 30,000 years (this general corrosion duration does not consider the 5 cm of stainless steel beneath the Alloy 22). While general corrosion occurs gradually over time up to the time of failure, the oxidation process is a surface phenomenon, and the underlying metal retains its integrity and resistance to drilling. Although TSPA-SR results show failures at early time, these failures are the result of localized corrosion and are not associated with degradation of the overall structural integrity of the waste package, and the resistance to drilling is maintained.

Waste Package Penetration by Drilling–There are a number of operational parameters that would indicate to a driller that down-hole conditions had changed and merit additional investigation and possibly a bit run (the removal of the bit from the hole for review and grading). A factor of two change in the rate of penetration or torque would be sufficient to indicate a change in drilling conditions and prompt additional investigations leading to the recognition that the driller had inadvertently drilled into a metallic material (i.e., drip shield or waste package).

The following discussion presents several lines of evidence relevant to estimating the time when a human intrusion could occur based upon the earliest time that current technology and practices could lead to waste package penetration without a driller noticing waste package penetration as being after the 10,000 year regulatory period.

The initial selection of bit type is typically made on the basis of what is known about the formation characteristics. The terms usually used by drilling engineers to describe the formation characteristics are drillability and abrasiveness. The drillability of the formation is a measure of how easy the rock formation is to drill. It is inversely related to the compressive strength of the rock, although other factors are also important. The abrasiveness of the formation is a measure of how rapidly the cutting surface of a bit will wear when drilling the formation. Although there are some exceptions, the abrasiveness tends to increase as the drillability decreases (Bourgoyne et al. 1986 [DIRS 155233]).

The bases for these discussions are typical practices used in drilling water wells in southwestern United States. The International Association of Drilling Contractors (IADC 1992 [DIRS 155232]) has developed a classification chart for selection of roller bits. Using this classification chart, roller bits with characteristics of 7-1 or 7-2 (hard semi-abrasive and abrasive formations) would be selected for drilling through the welded geologic units at Yucca Mountain, based on geo-mechanical properties. The 7-1 roller drill bits utilize 80 to 90 degree short chisel tungsten-carbide inserts, whereas the 7-2 roller drill bits utilize 60 to 70 degree short projectile tungsten-carbide inserts. Roller bits are typically used in drilling water wells due to their low cost and wide range of operational flexibility. Polycrystalline diamond cutter and diamond cutter drag bits typically are not used in water well drilling because of the high costs of these drill bits. Direct circulation hammer drills are sometimes used to drill brittle competent rock such as welded volcanic tuff, but they typically are inefficient in unconsolidated alluvium or incompetent rock formations. This limitation reduces the use of these drills in typical water well drilling. However, the discussions provided herein would be generally applicable to roller or hammer bits.

Uniaxial compressive strengths for the major geologic units at Yucca Mountain were determined using confined compression tests (Table A-1). Static Young's Modulus values were computed from stress-strain data obtained from unconfined compression tests. The intact rock unconfined compressive strength and elastic modulus by rock unit are given in Table A-1.

Based on the design described in the *Yucca Mountain Science and Engineering Report* (DOE 2001 [DIRS 153849]), Titanium grades 7 and 24 are candidate materials for drip shield fabrication and Alloy 22 and 316 nuclear grade stainless steel are candidate materials for waste package fabrication (DOE 2001 [DIRS 153849] Sections 2.4.4 and 3). Physical and chemical properties for these materials have been determined, and the tensile strength and modulus of elasticity for candidate drip shield and waste package materials are shown in Table A-2.

There have been a number of studies conducted to correlate operational parameters to rate of penetration of the drill bit. Many of these studies indicate that the rate of penetration is inversely proportional to the square of the compressive strength of the material being drilled, all other factors being equal (Bourgoyne et al. 1986 [DIRS 155233]; Warren 1987 [DIRS 155234]). This would indicate that a change of approximately 1.4 in the compressive strength of the material would be adequate to produce the factor of two change in the rate of penetration necessary for recognition by a driller.

Roller bits are designed to take advantage of brittle failure of the rock matrix to crush, break, and remove rock in an efficient manner. The volume of rock that is newly fractured by a tooth depends on the geometry, rock properties, and tooth penetration depth below the rock surface. The force applied to the tooth for a particular situation determines the tooth penetration depth. The bit tooth always penetrates into the rock until the resistant force offered back by the rock equals the force applied to the tooth. The tooth penetrates until the shear stress on the tooth caused by the weight on the bit is balanced by the shear strength of the rock. The rock may also become more ductile so that a greater tooth penetration is required to cause sufficient strain for chipping to occur (Warren 1987 [DIRS 155234]). As a load is applied to a bit tooth, the pressure beneath the tooth increases until it exceeds the crushing strength of the rock and a wedge of finely powered rock then is formed beneath the tooth. As the force of the tooth increases, the material in the wedge compresses and exerts high lateral forces on the solid rock surrounding the wedge until the shear stress exceeds the shear strength of the solid rock and the rock fractures. These fractures propagate along a maximum shear surface. As the force of the tooth increases above the threshold value, subsequent fracturing occurs in the region above the initial fracture, forming a zone of broken rock. The bit tooth moves forward until it reaches the bottom of the crater, and the process repeats (Bourgoyne et al. 1986 [DIRS 155233]).

The failure mechanisms between brittle rock and ductile steel differ significantly. The ductility of a material, usually measured as the percent reduction in area or elongation that occurs during a tensile test, can provide indications on how a material will fail. Ductile materials, with a minimum elongation in tensile testing, will not fail in service through brittle fracture (ASM 1997 [DIRS 155318]).

Selection of a bit for drilling involves knowledge of the characteristics of the rock. As indicated in Tables A-1 and A-2, there are differences between the tensile strengths and ductility of the geologic units at Yucca Mountain and the candidate materials for the drip shield and waste package. Because the materials used in the drip shield and waste packages have high compressive strengths and high ductility, the tooth of a roller bit cannot penetrate enough to cause sufficient strain for chipping to occur, resulting in a tearing action with associated high torque values. Bits designed for drilling rock would not be efficient for drilling through metal; boring in metals typically utilizes a milling technique. Milling produces a different failure mechanism than brittle failure that roller bits and hammer bits typically produce.

Bit operating conditions–Bit operating conditions (i.e., bit weight and rotary speed) affect the rate of penetration and the vibrations felt on the drill rig. The bit operating conditions affect and are affected by the rounded geometry of the emplacement drift, drip shield, and waste package, and size, orientation, and location of where the drilling assembly enters the emplacement drift and contacts the drip shield and waste package.

The loss of circulation of the drill and the sudden drop in weight when the drill bit breaks through the top of the emplacement drift would provide indications that conditions had changed. However, the lithophysal and fractured nature of certain of the Topopah Spring Tuff rock units could provide similar indications. Bit stabilization would be reduced as a result of the free space provided by the size of the emplacement drift (5.5 m) and the space between the crown of the emplacement drift and the drip shield and waste package if the drifts remain stable. A key block analysis has been performed to provide an indication of ground stability and the level of ground support necessary to keep repository openings stable during the operational period. This analysis indicates a block volume of approximately 0.1 cubic meters, at a 75 percent cumulative frequency of occurrence, would fall into the emplacement drifts should the drifts collapse (CRWMS M&O 1999 [DIRS 102111]). These relatively small rocks would tend to move or shift under small loads and the uneven loading on the drill bit would increase the lateral deviation forces by a phenomenon called preferential chip formation (Bourgoyne et al. 1986 [DIRS 155233]). As such, even if the drifts collapse the character of the rubble would be insufficient to stabilize the drill string. Severe wobbling bit action results as the bit is rotated if the drill collars or stabilizers above the bit are not held in a concentric position in the borehole.

The drilling assembly would have to contact the relatively small areas that make up the apex of the drip shield or waste package, where the surfaces are essentially perpendicular to the drill bit in order to have any possibility of penetrating these barriers. Lateral deviation forces increase with relatively small changes in the contact angle between the bit and the drilled material (Bourgoyne et al. 1986 [DIRS 155233]). Only the apex of the drip shield or waste package provides a perpendicular plane for which drip shield and waste package geometry would not increase the lateral deviation forces. If the drilling assembly contacted any location other than the relatively small areas that make up the apex of the drip shield or waste package, the combination of the large lateral deviation forces, the relatively small drill bit diameter and high rotational speeds, the lack of drill bit insert penetration and uneven loading on the bit (preferential chip formation), the high compressive strengths of the material used in the drip shield and waste package, and the lack of drilling assembly stability would likely cause the drill bit to slip off of the drip shield or waste package. Any penetration of the waste package or instability would be accompanied by a noticeable increase in drill string torque and reduced rate of penetration as the bit teeth contacted the metal. This increased torque would exacerbate the instability and increase the likelihood of the bit sliding past the metal. The chatter (vibration) resulting from the assembly bouncing on the top or side of these barriers would likely cause the drilling operator to change parameters in an attempt to smooth out operations.

Conclusion–The information presented in this appendix addresses the issue of when a human intrusion could occur based upon the earliest time that current technology and practices could lead to waste package penetration without the driller noticing waste package penetration. Conclusions based on information presented in this appendix suggest that a human intrusion event, if it were to occur, would not happen in the timeframe of regulatory compliance. The time to general corrosion failure of waste packages is approximately 30,000 years. Before this time, the presence of steel will be recognizable to the drillers, generally through loss of rate of penetration. This conclusion is conservative, because it is based on comparisons related to strength of the rock and steel and does not consider the 5 cm of stainless steel underneath the outer material of Alloy 22. The ductility of the metals makes them nearly impenetrable by techniques used in drilling rock, and the milling techniques needed to bore steel are not used in rock drilling, unless required for fishing operations or other specialized applications.

The elevation of the mountain and the resultant greater depth to water, especially when compared to shallower wells that would be required to the south of the mountain, make exploration unlikely. However, the regulations specify consideration of a human intrusion event. The TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) considered a stylized event occurring at 100 years, as specified in the proposed NRC regulation 10 CFR Part 63 (64 FR 8640 [DIRS 101680]). The TSPA-SR also examined the mean human intrusion annualized dose from an intrusion at 10,000 years. Both of these evaluations show that performance is within the regulatory limits.

Table A-1. Uniaxial Compressive Strength and Young's Moduli by Rock Unit

Rock Unit		Uniaxial Compressive Strength Mean [MPa]/Range	Elastic (Young's Modulus) Mean [GPa]
Tiva Canyon (welded)		127.5/36.0 to 230.9	29.4
Paintbrush Tuff (non-welded)		6.4/1.3 to 19.3	2.5
Topopah Springs (welded 1)		58.2/26.7 to 65.2	20.4
Topopah Springs (welded 2)		167.9/103.8 to 187.5	33.0
Proposed Repository Unit	Tptpmn	187.5	32.9
Proposed Repository Unit	Tptpll	103.8	27.5
	Tptpln	144.4	35.5
Topopah Springs (welded 3)		16.4/16.4	37.4
Calico Hills (non-welded)		23.2/20.5 to 24.6	5.6

Source: DTN: MO0003RIB00079.000 [DIRS 148295].

Table A-2. Candidate Material Properties for Drip Shield and Waste Package Fabrication

Engineered Barrier Material	Use	Tensile Strength [MPa]	Modulus of Elasticity [GPa]
Titanium Grade 7[a]	Drip Shield	345	106.9
Titanium Grade 24	Drip Shield	895[d]	113.8[e]
Alloy 22[b]	Waste Package	802	206
Type 316 Nuclear Grade Stainless Steel[c]	Waste Package	550	196

Source: [a] DTN: MO0003RIB00073.000 [DIRS 152926].
[b] DTN: MO0003RIB00071.000 [DIRS 148850].
[c] DTN: MO0003RIB00076.000 [DIRS 153044].
[d] Tensile Strength for Titanium Grade 24 (ASM International 1990 [DIRS 141615]).
[e] Modulus of Elasticity for Titanium Grade 24 (ASME 1998 [DIRS 145103]).

NOTE: Candidate materials based on the design described in the Yucca Mountain Science and Engineering Report (DOE 2001 [DIRS 153849], Sections 3.4 and 2.4.4).

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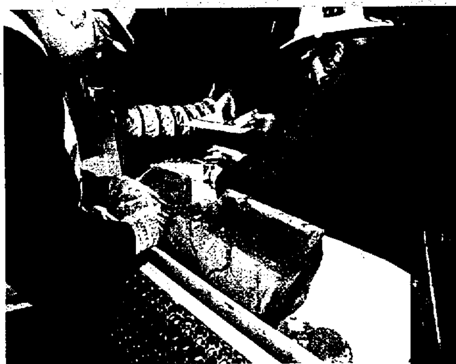

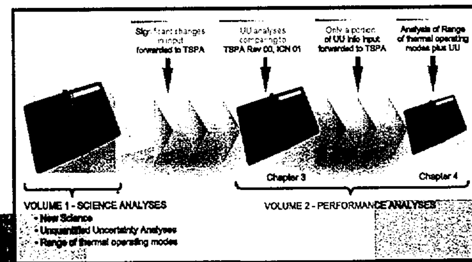
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