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Civilian Radioactive Waste Management System
Management & Operating Contractor

Comment Response on the Final Report: Peer Review of the Total System Performance Assessment–Viability Assessment (TSPA-VA)

B00000000-01717-5700-00037 REV 01

August 1999

Prepared for:

U.S. Department of Energy
Yucca Mountain Site Characterization Office
P.O. Box 30307
North Las Vegas, Nevada 89036-0307

Prepared by:

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Under Contract Number
DE-AC08-91RW00134

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ACKNOWLEDGMENTS

The evaluation of the findings and recommendations in the *Final Report Total System Performance Assessment Peer Review Panel* (Whipple et al. 1999) required input from across the Management and Operating Contractor and the U.S. Geological Survey. Principal contributors to the evaluation included: Robert Andrews, Robert Dulin, Joon Lee, Yueting Chen, James Houseworth, Jerry McNeish, David Sassani, David Sevougian, and Eric Siegmann (Duke Engineering & Services Company); David Stahl (Framatome Cogema Fuels); Phillip Oberlander and Ardyth Simmons (Lawrence Berkeley National Laboratory); James Blink and Thomas Buscheck (Lawrence Livermore National Laboratory); Paul Dixon (Los Alamos National Laboratory); William Arnold, Ralston Banard, Holly Dockery, Cliff Ho, Nicholas Francis, Robert MacKinnon, Rob Rechard, and Mike Wilson (Sandia National Laboratories); Jeff Tappen (Science Applications International Corporation); John Gauthier (Spectra Research, Inc.); Al Eddebbarh and Robin Datta (URS Greiner Woodward Clyde); and Dwight Hoxie (U.S. Geological Survey).

We have also benefited from the thoughtful reviews and suggested modifications of the draft integrated version of this document from Jerry McNeish (Duke Engineering & Services Company); David Stahl (Framatome Cogema Fuels); Richard Snell (Fluor Daniel); Donald Watkins and Michael Voegele (Science Applications International Corporation), Ann Schaeffer (Science & Engineering Associates), Jack Bailey, Larry Rickertsen, and Mark Wisenburg (TRW Environmental Safety Systems, Inc.); and Dwight Hoxie (U.S. Geological Survey).

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OVERVIEW

The Management and Operating Contractor established a Performance Assessment Peer Review Panel (hereinafter "the Panel") at the request of the U.S. Department of Energy Yucca Mountain Site Characterization Office. The objectives of the peer review were to provide:

- A formal, independent evaluation and critique of *Viability Assessment of a Repository at Yucca Mountain: Total System Performance Assessment, Volume 3* (DOE 1998a; hereinafter "Total System Performance Assessment-Viability Assessment") that was conducted in support of the *Viability Assessment of a Repository at Yucca Mountain* (DOE 1998b)

- Suggestions for improvements as the U.S. Department of Energy prepares to develop the documentation for a Total System Performance Assessment to support a potential License Application

The Panel conducted a phased review over a two-year period to observe the development and, ultimately, to review the Total System Performance Assessment-Viability Assessment (DOE 1998a). During the development of the Total System Performance Assessment-Viability Assessment (DOE 1998a), the Panel submitted three Interim Reports (Whipple et al., 1997a, 1997b, and 1998) to the Management and Operating Contractor with recommendations and comments on the process models, model abstractions, and draft documentation for the Total System Performance Assessment-Viability Assessment (DOE 1998a).

The Panel's *Final Report Total System Performance Assessment Peer Review Panel* (Whipple et al. 1999; hereinafter "Final Report") on the Total System Performance Assessment-Viability Assessment (DOE 1998a) is based primarily on the completed Total System Performance Assessment-Viability Assessment (DOE 1998a), the *Total System Performance Assessment-Viability Assessment* (TSPA-VA) *Analyses Technical Basis Document* (CRWMS M&O 1998), and the cited references. The Final Report (Whipple et al. 1999) includes the major points from the three Interim Reports (Whipple et al. 1997a, 1997b, and 1998), updated where appropriate, as well as new findings that the Panel developed during its review of the Total System Performance Assessment-Viability Assessment (DOE 1998a).

In the Final Report (Whipple et al. 1999), the Panel notes that the objective of the Total System Performance Assessment-Viability Assessment (DOE 1998a) was to describe the probable behavior of the potential repository. The Panel states that because of the mixture of analyses (some intended to be conservative and some intended to be realistic), the Total System Performance Assessment-Viability Assessment (DOE 1998a) "*cannot be viewed as an accurate projection of the probable behavior of the site.*" The Panel also states that it is not likely that the Total System Performance Assessment-Viability Assessment (DOE 1998a) describes the probable behavior of the potential repository system. They do, however, consider the analysis to be a useful step in evolving the understanding of how a repository could be expected to perform at Yucca Mountain.

The Management and Operating Contractor does not agree with the Panel's position that "*it is unlikely that the* [Total System Performance Assessment-Viability Assessment], *taken as a whole, describes the long-term probable behavior of the system.*" The Management and Operating Contractor believes that the Total System Performance Assessment-Viability Assessment (DOE 1998a) analyzed the long-term probable behavior of the repository system and that this behavior is likely captured within the range of results presented in the Total System Performance Assessment-Viability Assessment (DOE 1998a). The Total System Performance Assessment-Viability Assessment (DOE 1998a) was not intended to provide a precise projection of the probable behavior of the potential repository system. It was intended to provide the probable behavior of the potential repository system as a snapshot in time, given the available information and analyses, and the design concepts for the Viability Assessment design (DOE 1998b).

The Panel also noted that the Total System Performance Assessment-Viability Assessment (DOE 1998a) "*has been useful in identifying aspects that are comparatively unimportant to performance, for which additional data and analyses are not likely to be beneficial.*" The Management and Operating Contractor concurs that the Total System Performance Assessment-Viability Assessment (DOE 1998a) has helped to identify aspects of the repository system for which additional data and analyses will not be beneficial.

The Panel goes on to state that the objective of Total System Performance Assessment-License Application will be to determine if it can be shown that the repository will comply with the applicable regulatory limits with reasonable assurance rather than to describe the probable behavior of the potential repository system. The Panel considers this objective to be significantly different from the objective of the Total System Performance Assessment-Viability Assessment (DOE 1998a) and recommends approaches for achieving it.

The Panel identifies two types of processes that need to be analyzed for the potential License Application: 1) processes for which analytical models are available, and 2) processes that may be intractable, given current analytical capabilities or current time constraints.

The Panel suggests five approaches to address these processes:

- Updating component models
- Expanding the quality and quantity of data for analyses
- Using bounding assumptions
- Making design changes
- Incorporating the defense-in-depth concept

On page 44 of the Final Report (Whipple et al. 1999), the Panel also states:

> *For cases in which it is feasible to improve either the component models or their underlying data, the Panel recommends that efforts be made to implement such improvements wherever such changes would affect the overall assessment. Where conservative bounding analyses do not result in unduly pessimistic estimates of the total system performance, the Panel recognizes that it may not be cost-effective to spend additional time and effort refining the assessments and making them more*

realistic. For those issues for which, by virtue of their complexity, it is not feasible to produce more realistic models supported by data, the Panel recommends that a combination of bounding analyses and design changes be applied.

The Management and Operating Contractor concurs with these approaches. They are consistent with U.S. Department of Energy's strategy for developing a postclosure safety case for the potential Site Recommendation/License Application, with the ongoing License Application Design Selection process, and with U.S. Department of Energy's ongoing efforts to prioritize future work for the potential Site Recommendation/License Application.

In summary, the Panel has provided a thorough and thoughtful review of the Total System Performance Assessment-Viability Assessment (DOE 1998a). The Panel's overarching strategy for improving the Total System Performance Assessment-Viability Assessment (DOE 1998a) analysis is consistent with the U.S. Department of Energy's approach for developing the postclosure safety case for the potential Site Recommendation/License Application. In contrast, the Panel's specific comments on the limitations of the component models and the associated databases were provided in the context of the Total System Performance Assessment-Viability Assessment (DOE 1998a) and the Viability Assessment design (DOE 1998b). The Management and Operating Contractor has evaluated these comments in the context of the ongoing License Application Design Selection process and efforts to re-prioritize future work. The relative importance of the Panel's specific comments will depend on the U.S. Department of Energy's selection of a design for the potential Site Recommendation/License Application and the evolution of the U.S. Department of Energy's postclosure safety case. The Management and Operating Contractor will consider these specific comments for the development of the Total System Performance Assessment-Site Recommendation/License Application in the context of the design that is selected for Site Recommendation/License Application and the evolving postclosure safety case.

This report documents the comments provided in the Final Report (Whipple et al. 1999) and the Management and Operating Contractor responses to these comments. The responses were based on input from a number of scientists from the Management and Operating Contractor, several national laboratories, and the U.S. Geological Survey. The comments and responses are organized to be consistent with the major headings in the Final Report (Whipple et al. 1999). Excerpts from the Final Report (Whipple et al. 1999) are in italics; the Management and Operating Contractor responses to the comments are in straight text.

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ACRONYMS AND ABBREVIATIONS

AMF	Air-Mass Fraction
CAM	Corrosion-Allowance Material
CRM	Corrosion-Resistant Material
CRWMS	Civilian Radioactive Waste Management System
DOE	U.S. Department of Energy
DSNF	Defense Spent Nuclear Fuel
EBS	Engineered Barrier System
ESF	Exploratory Studies Facility
EPA	U.S. Environmental Protection Agency
EWCD	East-West Cross Drift
EWDP	Early Warning Drilling Program
HLW	High-Level Waste
LA	License Application
LADS	License Application Design Selection
M&O	Management and Operating Contractor
NFE	Near-Field Environment
NFGE	Near-Field Geochemical Environment
NRC	Nuclear Regulatory Commission
NSNFP	National Spent Nuclear Fuel Program
NTS	Nevada Test Site
PMR	Process Model Report
SCC	Stress Corrosion Cracking
SR	Site Recommendation
SZ	Saturated Zone
TH	Thermal-Hydrologic
THC	Thermal-Hydrologic-Chemical
TSPA	Total System Performance Assessment
TSPA TBD	Total System Performance Assessment Technical Basis Document
TSPA-LA	Total System Performance Assessment-License Application
TSPVA-SR	Total System Performance Assessment-Site Recommendation
TSPA-SR/LA	Total System Performance Assessment-Site Recommendation/ License Application
TSPA-VA	Total System Performance Assessment-Viability Assessment

UZ	Unsaturated Zone
VA	*Viability Assessment of a Repository at Yucca Mountain* (DOE 1998b)
WAPDEG	A computer software code developed to model long-term corrosion degradation of waste disposal containers in the potential repository.
2-D	Two-Dimensional
3-D	Three-Dimensional

1. MAIN FINDINGS

The Performance Assessment Peer Review Panel (hereinafter "the Panel") conducted a phased review over a two-year period to observe the development and, ultimately, to review the *Viability Assessment of a Repository at Yucca Mountain: Total System Performance Assessment, Volume 3* (DOE 1998a; hereinafter "TSPA-VA") that was conducted in support of the *Viability Assessment of a Repository at Yucca Mountain* (DOE 1998b; hereinafter "VA"). During the development of the TSPA-VA (DOE 1998a), the Panel submitted three Interim Reports (Whipple et al. 1997a, 1997b, and 1998) to the Management and Operating Contractor (M&O) with recommendations and comments on the process models, model abstractions, and draft documentation for the TSPA-VA (DOE 1998a).

The Panel's final report on the TSPA-VA (DOE 1998a), *Final Report Total System Performance Assessment Peer Review Panel* (Whipple et al. 1999; hereinafter "the Final Report") is based primarily on the completed TSPA-VA (DOE 1998a), the *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document* (CRWMS M&O 1998; hereinafter "TSPA-VA TBD"), and references cited in these reports. The Final Report (Whipple et al. 1999) includes the major points from the three Interim Reports (Whipple et al., 1997a, 1997b, and 1998), updated where appropriate, as well as new findings that the Panel developed during its review of the TSPA-VA (DOE 1998a).

The Panel provided a thorough and thoughtful review of the TSPA-VA (DOE 1998a). The Panel's overarching strategy for improving the TSPA-VA (DOE 1998a) analysis is consistent with the U.S. Department of Energy's (DOE) approach for developing the postclosure safety case for the potential Site Recommendation/License Application (SR/LA). In contrast, the Panel's specific comments on the limitations of the component models and the associated databases were provided in the context of the TSPA-VA (DOE 1998a) and the VA design (DOE 1998b). The M&O has evaluated these comments in the context of the ongoing License Application Design Selection (LADS) process and efforts to re-prioritize future work. The relative importance of the Panel's specific comments will depend on the DOE's selection of a design for SR/LA and the evolution of the DOE's postclosure safety case. The M&O will consider these specific comments for the development of the TSPA-SR/LA in the context of the design that is selected for SR/LA, if the site is found suitable, and the evolving postclosure safety case.

The following sections document the comments provided in the Final Report (Whipple et al. 1999) and the M&O response to these comments. The responses were based on input from a number of scientists from the M&O, several national laboratories, and the U.S. Geological Survey[1]. The comments and responses are organized to be consistent with the major headings in the Final Report (Whipple et al. 1999). Excerpts from the Final Report (Whipple et al. 1999) are in italics; the M&O responses to the comments are in straight text.

[1] See Acknowledgments.

1.1 RELIABILITY OF THE TSPA-VA RESULTS

Comment 1 (pages 15–16): *Because of the inadequacy of the supporting evidence, the Panel could not confirm whether a number of the TSPA-VA component models are representative of the systems, components, and processes they were designed to simulate. In addition, several of the component models are likely to be conservative and others non-conservative. For these reasons, it is unlikely that the TSPA-VA, taken as a whole, describes the long-term probable behavior of the proposed repository....*

The objective for the TSPA-VA was to assess the probable behavior of the repository. In contrast, the objective for the TSPA-LA will be to determine whether it can be shown with reasonable assurance that the repository complies with the applicable regulatory limits. These are significantly different objectives, and recognition of this distinction should be an important element of a path forward to the TSPA-LA. This issue is discussed in more detail in Section III.

Response: The M&O does not agree with the first part of this comment. The TSPA-VA (DOE 1998a) was not meant to be a definitive prediction of probable repository behavior. Although the M&O agrees that the representations of the various component models are uneven in their degree of maturity, the analyses have incorporated the available scientific data and the VA design (DOE 1998b) concepts for the repository and the waste package. The M&O has also incorporated the most current understanding of key processes affecting the long-term behavior of the potential repository system. In this description of the probable behavior of the repository system, the M&O acknowledges that these evaluations are uncertain. Several factors lead to this uncertainty, including:

- The long time frame of the analyses
- The heterogeneous site
- The coupled system
- The unknown future populations

Although these uncertainties are recognized in the analyses and the interpretations of these analyses, they do not detract from the goal to objectively evaluate how the system is likely to behave. For the TSPA-VA (DOE 1998a), the M&O completed a deterministic case and a fully probabilistic case. Multiple realizations were used to define the range in the dose rates. The M&O believes that TSPA-VA (DOE 1998a) analyzed the long-term probable behavior of the repository system and that this behavior has likely been captured within the range of results presented. That range, however, is large. The goal for the upcoming cycle of TSPAs is to decrease the range of values and to gain more confidence in the median of the distribution.

The M&O agrees with the second part of this comment. The objectives of the TSPA-LA will be more stringent, focusing on demonstrating compliance with regulatory requirements. The M&O also agrees with the Panel's suggested approach for a path forward towards a potential LA. This approach (Whipple et al. 1999) includes:

- Updating component models
- Expanding the quality and quantity of data for analyses
- Using bounding analyses

- Making design changes
- Incorporating defense-in-depth concepts into the design for SR/LA

The M&O is implementing the suggested steps for a more robust TSPA-SR/LA. New data and refined analyses will be used to help constrain the range of values and increase confidence in the system performance. In addition, the selection of a design for SR/LA will focus on design changes and bounding analyses, where appropriate, to improve system performance. The M&O will also evaluate the design margin, defense-in-depth, and the performance confirmation program to enhance confidence that the potential repository system will meet regulatory requirements.

Comment 2 (page 15): *With the benefit of hindsight, the Peer Review Panel finds that a credible assessment of the future probable behavior of the repository is beyond current analytical capabilities, given the complexity of the system and the nature of the data that now exist or that could be obtained within reasonable time and cost. The TSPA-VA team has performed well, has developed numerous analytical innovations, and has produced technical reports of exemplary clarity. The failure of the TSPA-VA to capture the probable future behavior of the proposed repository system is due in large part to the difficulty of the problem, including the long time scales over which performance is to be described and the large and heterogeneous physical setting that is addressed by the analysis. This difficulty was compounded by a failure, in many elements of the analyses, to initiate and complete the necessary research, develop the appropriate models, and collect and apply the needed data and information.*

Response: The M&O does not agree that a credible assessment of the probable future behavior of the potential repository is beyond current analytical capabilities. Since the Yucca Mountain Site Characterization Project started, the M&O has obtained considerable information on the site and has gained a great deal of knowledge about how the natural systems operate. Many of the models that the M&O can now validate with laboratory and field data represent major steps forward in the development of those technical fields. However, the M&O agrees that more information is needed in some areas. The DOE is refining the postclosure safety case to help understand which information contributes the greatest uncertainty to the dose estimates in order to prioritize information-gathering activities. In this way, the M&O can most effectively determine when to obtain additional information and when to simply utilize the available data and develop appropriate models.

Comment 3 (page 15): *Until there are improvements in the specific subsystem models for key elements of the system, in their supporting databases, in the coupling between certain aspects of the modeling, and in the use of tests, overall conclusions based on the analyses should be viewed skeptically, and decisions based on the analyses should be made cautiously.*

Response: The M&O agrees and is working to collect additional data and to improve the models, the data, and their documented justification for the potential SR/LA.

Comment 4 (page 16): *The Panel recognizes that substantial amounts of field and experimental data have been developed in support of the TSPA-VA; to be credible, however, many elements of the analysis require additional data. These data needs are of two types: fundamental data that*

are essential to the development and implementation of the models, and data sets designed to challenge conceptual models and test the coupled models used in the TSPA-VA.

Response: The M&O agrees and is actively collecting data that are essential for model development and to test models. The types of information to be obtained for the TSPA-SR/LA will be determined by the DOE's evolving postclosure safety case for SR/LA. The needs identified in the Issue Resolution Status Reports issued by the U.S. Nuclear Regulatory Commission (NRC), formal comments from the Nuclear Waste Technical Review Board, and recommendations presented by this Panel will be considered in the development of the postclosure safety case for SR/LA. The objective of the ongoing prioritization is to establish the relative importance of the necessary data and analyses.

Comment 5 (pages 16–17): *To be credible, the analysis would have needed to include:*

- *Component subsystem models that capture important and relevant phenomena;*
- *Adequate databases;*
- *Proper coupling between the subsystem models; and*
- *Tests of modeled behavior.*

Although the TSPA-VA offers many examples of partial, even substantial, success in each of these four areas, the Panel has also observed examples of important deficiencies in each.

- *Concerning subsystem models, the final dose estimates within the TSPA-VA rest in large part on potentially optimistic, or at least undemonstrated, assumptions about the behavior of certain barriers in the system (for example, performance of the cladding and the waste package).*

Response: With respect to cladding, the M&O is currently reviewing the best estimates for cladding failure and the ranges that will be used in the potential LA, as the ranges for the cladding analysis may have been too narrow for TSPA-VA (DOE 1998a). For example, the fraction of cladding damaged during reactor operation was 0.1 percent, without considering the ranges. A more detailed review of the operating history for boiling water reactors shows that there is a 1 percent chance that fuel could have over 2.5 percent rod perforation, based on waste packages loaded with certain cores from the mid-1970s. Future analysis will provide a better basis for both the best estimates and ranges.

With respect to the waste package degradation analysis, where no process-level information was available, conservative (or bounding) assumptions were employed. For example, the M&O took conservative approaches in modeling the likelihood and penetration rate of crevice and pitting corrosion of the Alloy 22 inner barrier. Specific examples of the conservative approaches to the crevice and pitting corrosion modeling include:

- 100 percent probability of crevice formation under dripping conditions after breach of the carbon steel outer barrier

- Critical threshold temperature for initiation, assuming aggressive crevice solution chemistry inside the crevice

- Pitting corrosion with penetration rates from a range of solution chemistries, including highly aggressive conditions, after corrosion initiation

- Pits inside crevices continue to grow after initiation of corrosion

Pit stifling or pit repassivation that is likely to occur during the penetration of a thick layer of a highly corrosion-resistant alloy, such as Alloy 22, was not considered. For general corrosion of the Alloy 22 inner barrier, the same penetration rates sampled for the patches were used for the entire simulation period. That is, the analysis did not consider the potential for decreasing general corrosion rates that could result from changes in the exposure (water chemistry) conditions on the waste package surface to less corrosive conditions over time. In reality, a decrease in the general corrosion rate is likely from a limited concentration of aggressive species from sustained dripping on the waste package surface and the high humidity in the drifts.

Potential non-conservatism in the waste package degradation analysis is acknowledged by not including: 1) stress corrosion cracking (SCC) of the Alloy 22 inner barrier, and 2) the effect of potential stress generation from volume expansion of carbon steel corrosion product oxides in the crevice between the two barriers (CRWMS M&O 1998). Their impacts are uncertain at the present time, and detailed analysis and testing are needed to quantify their impacts on waste package degradation. Also, additional data and analysis are needed to substantiate and/or update the modeling assumptions used for the individual degradation processes employed in the waste package degradation analysis.

- *Concerning databases, some of the important analyses are not supported by an adequate database, (for example, databases for the corrosion of spent fuel and the saturated zone analysis).*

Response: The M&O has utilized available information from the literature to support its position and to provide support for models for the corrosion of spent fuel. This approach was adequate for the VA (DOE 1998b). However, for the potential SR and LA, qualified data will be utilized as the basis for the development of predictive models. Data from the literature will be utilized as corroborative information. This has already been done for the dissolution rate of uranium oxide and spent fuel. For Alloy 22, where corrosion data are limited due to its relatively recent introduction, the corrosion performance will be compared to precursor nickel-based alloys that are not as corrosion resistant, but for which a larger database exists.

The Early Warning Drilling Program (EWDP) being undertaken by Nye County is expected to enhance the hydrogeologic data set needed for input to the site-scale saturated zone (SZ) flow and transport model in the down-gradient alluvial-aquifer segment of the expected pathway to the accessible environment. Laboratory experiments are being performed to provide additional data on neptunium speciation and solubility, and to improve assessments of colloid-facilitated transport. Laboratory experiments also are being performed, in addition to the collection of data from the ongoing Drift-Scale Heater Test, to enlarge the database by which to test and calibrate models simulating coupled thermal, hydrologic, and chemical processes within the rock mass enclosing the potential repository. The Busted Butte Field Test is expected to enhance

knowledge of the flow and transport processes and the hydrologic- and transport-property data sets needed to evaluate radionuclide transport through the Calico Hills nonwelded hydrological unit in the unsaturated zone (UZ) beneath the repository.

- *Concerning coupled processes (that is, thermohydrological, thermomechanical, and thermochemical effects) and the data and models that support them, the Panel believes that it may be beyond the capabilities of current analytical methodologies to analyze systems of such scale and complexity. For this reason, the effects of coupled processes can probably best be dealt with through a combination of bounding analyses and engineered features designed to minimize the effects of such processes.*

The M&O is evaluating the recommended approach to analyzing coupled processes. Lower thermal loads (which would reduce the effects of coupled processes) are being considered in the LADS process, though no decision has yet been made. First, rather than attempting to calculate specific thermal-hydrologic-mechanical-chemical effects at fine spatial and temporal scales, the M&O has used geostatistical methods and nested-scale models to bound the effects. Second, the LADS process has emphasized the use of engineered features that are designed to minimize coupled-process effects. The designs that are being considered include a reduced areal mass loading and enhanced preclosure thermal management features compared to the VA (DOE 1998b). These designs result in the boiling fronts penetrating only a few meters into the very wide pillars between drifts, and the duration of temperatures above the boiling point of water will only be several centuries. Thus, coupled processes in the rock would be much less significant to performance than for the VA design (DOE 1998b). Finally, the use of drip shields and optional backfill reduce the probability of crevice corrosion and pitting of the waste packages by avoiding the temperature–relative humidity windows of susceptibility for these modes and by diverting seepage water away from the waste packages.

The M&O expects that the Drift-Scale Heater Test will be quite valuable in terms of "verifying" the thermal response models. At the same time, the Panel's suggestion to consider bounding analyses is being pursued as well. It may be difficult to truly "bound" the effects of coupled processes, but in the TSPA-VA (DOE 1998a), sensitivity analyses were "bounded," to some extent, where the effects of coupled processes were likened to the effects of larger or smaller fracture apertures for seepage into the drifts.

- *Concerning tests of modeled behavior, the TSPA-VA does not contain the convincing direct measurements or confirmation of the modeled behavior of components or subsystems for which testing is feasible. This testing should be a part of the analyses of such a complicated system.*

Response: The site-scale UZ flow and transport model is being tested in a number of ways, including predictions of and comparisons against ambient geochemistry and perched-water distributions within the UZ, pneumatic responses monitored in boreholes, temperature profiles measured in boreholes, and hydrologic conditions within the East-West Cross Drift (EWCD). Coupled thermal, hydrologic, and chemical models are being tested against the results from laboratory experiments, as well as against data acquired from the Large Block Test, the Single Heater Test, and the Drift-Scale Heater Test. Both natural and anthropogenic analogue data will be used to the extent feasible to test both conceptual and numerical models.

Regarding the waste packages, long-term testing is continuing under expected service conditions and short-term tests are underway under accelerated conditions. This information, along with any applicable analogue data, can be used to test model performance predictions.

Comment 6 (page 17): *Depending on the degree of confidence that is necessary for licensing, the current analyses may not be adequate. As discussed in Section III, the Panel believes that, for many issues to be addressed in the TSPA-LA, use of simplified bounding analyses may be necessary to achieve the desired degree of confidence.*

Response: All of the models in the TSPA have been simplified to some extent. No model, no matter how detailed, can capture all of the details needed to completely describe the natural or engineered components. The goal of the iterative TSPA is to determine how much simplification can be achieved without losing important details or interrelationships. Therefore, the M&O certainly agrees that it is useful to pursue simplification, but only where the simplification can: 1) be demonstrated to be truly bounding, and 2) is such that the M&O can be certain that all important processes and interactions have been adequately captured.

1.2 ADVANCES AND IMPROVEMENTS IN THE TSPA-VA ANALYSIS

Comment 7 (page 18): *The Project team has incorporated a dramatic and needed improvement in numerical modeling in the area of transport in the saturated zone, where they have abandoned the previous finite-difference model in favor of a streamtube-based approach. Although the adoption of a streamtube approach based on an overall dilution factor is less desirable than a more detailed treatment of dispersion, it is appropriate, given the limitations in the data concerning the saturated zone. The new model eliminated numerical dispersion errors, inherent in the previous model, and may provide a more realistic prediction of dilution in the saturated zone. This model is not physically representative of the saturated zone transport for isolated waste package failures, however, although sensitivity analyses indicate that the model overestimates dilution for such cases by perhaps a factor of three. This factor is small in comparison to the other uncertainties in the assessment of the saturated zone.*

Response: The TSPA-VA (DOE 1998a) analyses for the SZ do underestimate the concentrations in the accessible environment for those times in which a single waste package is contributing radionuclides to the system. These times are near the beginning of the simulations and possibly impact calculated doses at 10,000 years, but probably have no impact on calculated maximum doses in the 100,000-year and 1-million-year simulations.

The approach for future TSPA modeling will use streamline particle-tracking methodology in a three-dimensional (3-D) flow and transport model. Use of the 3-D model will not require the implicit homogenization of the streamtube approach. The source size will be conservatively assigned to a small region (approximately 100 m x 100 m) that will not result in the overestimates of dilution inherent in the TSPA-VA (DOE 1998a) approach. Simulating a source region at the water table of less than 100 m x 100 m would not result in higher concentrations at 20 km for a given value of transverse dispersivity, as confirmed in a sensitivity analysis by Arnold and Kuzio (Memorandum, 1998).

1.3 KEY ROLE OF THE WASTE PACKAGE

Comment 8 (page 19): *A more rigorous treatment of the evaluation of the performance of the waste package material requires the determination of two important factors:*

- *The realistic, extreme environments expected to come in contact with the C-22 metal surface; and*
- *The critical temperature for crevice corrosion of C-22 in the presence of these environments.*

Response: There are ongoing efforts, both analytically and experimentally (the latter in the Drift-Scale Heater Test), to understand the change in water chemistry over time. The exposure conditions for the Long-Term Corrosion Test Facility tanks were established at the initiation of those experiments more than two years ago. At the time, a workshop consisting mainly of geochemists determined the expected composition range to be a 10 times J-13 water composition with pH values of 4.5 to 10. This was further expanded to pH 2.7 to 11 to take into account microbiological and concrete material impacts. The 1,000 times J-13 chemistry was selected as representative of very concentrated solutions due to evaporation. Recent work has focused on evaporation to dryness and the resultant equilibrium compositions at elevated temperature and high relative humidity. With these studies, the experimental program is attempting to bound the likely range of conditions and test the candidate waste package materials at these conditions.

A mechanistic process model was developed, based on observed phenomena published in the scientific literature and data developed by the M&O. The model can be used to predict the extent to which pH will be lowered and the extent to which the chloride anion concentration is increased. The predictions are based on experimentally determined hydrolysis equilibrium constants, experimentally determined cyclic polarization curves, and other experimental sources of data.

Crevice corrosion testing as a function of temperature, pH, oxidizing potential, and ionic species is underway. The kinetics of the relationships may or may not provide a sharp threshold, but should, under the conditions evaluated, indicate the temperatures below which crevice corrosion is negligible.

Comment 9 (page 20): *For the TSPA-VA, the critical temperature for localized corrosion of C-22 was estimated to be 80°C and the critical temperature for moisture formation was estimated to be 100°C. An estimated probability function was used for estimating the onset of localized corrosion once the package reaches the critical temperature range. Estimates of corrosion rates as a function of temperature were used to determine the corrosion damage (penetration depth). While the approach is sound, once again it is important to recognize that all of the estimates of crucial parameters were based upon expert elicitation, not upon experimental data.*

Response: The M&O is continuing to collect long-term and short-term data to improve the models to be used in subsequent TSPA analyses. Specific attention is being paid to the

collection of the crucial parameters. At the time of the LA, however, only five-year data will be available.

Comment 10 (pages 20–21): *The Panel considers the TSPA-VA to be a useful tool for better understanding the performance and the effects of individual components on the expected repository performance; however, the TSPA treats a highly complex system and is a work in progress. The Panel concludes that the results of the TSPA-VA should be used cautiously, and that they should not be used as the primary criterion for design selection. This is particularly relevant to the evaluation of engineering components and structures. For example, the outcomes of the TSPA-VA clearly show that preventing water coming into contact with the waste packages is highly beneficial. However, the projected efficacy of an additional engineered water barrier, be it a drip shield, backfill barrier, or ceramic coating, is driven by the assumptions made within the TSPA. The Panel concludes that many of these assumptions do not have an adequate analytical and experimental justification. In a similar manner, the credibility of the conclusions is dependent upon the underlying engineering and science that supports the presumed performance of the enhanced engineering features.*

Response: The M&O agrees that any specific numerical results used to make decisions related to the repository system must be used judiciously. However, as the Panel has noted, running models under ranges of conditions and input values can be used in conjunction with data and expert judgement to gain intuition about how the system might work. Before any of the specific design features can be used as part of a safety argument, the M&O will need to develop better models with a mechanistic basis and exercise them within the context of the subsystem models and the total-system model.

The LADS work over the past year has used performance assessment as a means of gaining insight into processes that could cause a design or the natural system to fail to meet regulatory criteria or design goals. The insights gained were used to develop design solutions that reduce reliance on uncertain models or that mitigate the consequences of uncertainties. Examples may include limiting the extent and duration of above-100°C temperatures in the rock, separating the drifts to make them less coupled from a computational perspective, using line loading and blending to reduce temperature variation along the drifts, and using drip shields and optional backfill to reduce the need to accurately predict seepage and rockfall.

The M&O agrees that the potential SR/LA will require more detailed data and models, backed by mechanistic understanding wherever possible. Focusing of future efforts on the selected LADS design will direct resources to these key areas.

Comment 11 (page 21): *For purposes of evaluating alternative design features, the Panel recommends that a concentrated effort be undertaken to collect and collate the available experimental data germane to an analysis of waste package performance.*

Response: The M&O agrees with the Panel recommendation. A review of available germane experimental data has been completed on titanium (Ti) alloy corrosion and on radiolysis effects on the corrosion of nickel-based, titanium-based, and stainless steel alloys. In addition, literature surveys of material degradation modes have been completed on relevant nickel-based, titanium-based, and stainless steel alloys.

1.4 KEY ROLE OF INFILTRATION AND SEEPS ANALYSIS

Comment 12A (page 22): *The Panel considers the analysis of seepage into drifts novel and informative. Given that it was only recently performed, however, it is understandable that the resulting analysis represents only a first-order approximation and that further improvements will be necessary before the accompanying estimates can be adopted with confidence. The following issues are of particular concern to the Panel.*

The analysis relies on a conventional but questionable van Genuchten formalism applied to a fracture continuum. This approach ignored the unstable nature of gravity-driven infiltration in real fractures, the possibility of hysteretic (and chaotic) behavior during episodic flow, as documented in recent experiments in related systems (Faybishenko et al. 1998), the discrete nature of the fracture network, and a detailed characterization of the capillary barrier condition at the drift surface. Thus, it is questionable that the representation assumed for purposes of developing the model actually reflects the true physics of seepage in a fractured system. Furthermore, the analysts ignored the possibility of drift collapse as a result of thermomechanical or seismic events, except for the analysis of waste package damage from rockfall.

Response: The experimental seepage program is intended to address these concerns, and the M&O should have a firmer basis for the seepage model for TSPA-SR/LA because of this work. Drift-collapse effects on seepage will be included in TSPA-SR/LA. Note, also, that DOE is sponsoring a Drift Seepage Peer Review to evaluate the sufficiency of the testing and modeling approaches.

The application of van Genuchten parameter fitting, which was developed for alluvial material, to fractures is based on laboratory moisture-retention data and it produces results that are consistent. There are no currently accepted alternatives to van Genuchten parameters in this application of coupled matrix and fracture modeling. The M&O is approaching this issue by examining modifications to the van Genuchten relationships that will be based on physical measurements.

Alternative drift geometries will be evaluated in the UZ Drift-Scale model to estimate the effects of partial drift collapse. The collapse features will be based on probable rockfall distributions and will assume that an air gap remains between the drift wall and the waste package. Asperities along the drift wall will increase the probability of a dripping flux.

Comment 12B (pages 22–23): *Because of the steady-state assumptions made, seep locations and rates are estimated to be time-independent, under conditions of constant climate. Specifically, the Project staff has assumed that water will come into contact with (drip onto) some patches some of the time, but water will not come into contact with other patches for periods as long as 1,000,000 years. Although a case was made in the TSPA-VA to support this assumption, the associated understanding of the features of the mountain, including the location and size of fractures, is not adequate. In addition, thermomechanical and thermochemical effects on the permeability and capillary structure of the fracture network will alter seepage patterns as a function of time, not only during the period of the thermal pulse, but also in a longer time horizon (recall that thermomechanical effects will last as long as the mountain is at*

a temperature higher than the ambient). This raises the possibility that seep locations and rates will shift with time. The consequences of this possibility should be investigated. Conversely, if precipitation caps develop (Hardin 1998), they may act to reduce the amount of seepage in drifts over which such a cap forms over a long time period. This effect was not considered in the TSPA-VA.

Response: In the TSPA-VA (DOE 1998a), the M&O assumed that seeps were stable over time with regard to which waste packages they contacted, but they were assumed to "wander" locally, so that the entire waste-package surface was wetted by the seep. The M&O agrees that this is an important assumption and that it needs to be investigated in the future. Similarly, if precipitate caps are determined to be a likely occurrence, their effects on seepage will need to be investigated.

Alternative drift geometries will be evaluated in the UZ Drift-Scale model to estimate the effects of partial drift collapse. The collapse features will be based on probable rockfall distributions and will assume that an air gap remains between the drift wall and the waste package.

Heterogeneity in the rock surrounding the drift wall is evaluated by stochastic variations in the hydraulic parameters describing flow in fractures. The distribution of air permeability values, which mainly characterize the fractures, will be used to describe the heterogeneity.

The overlying Paintbrush nonwelded unit will damp episodic infiltration from infiltration events. Episodic flow as a result of heating and reflux is believed to be a short-term condition that will take place between dry-out of the drift walls and repository cool-down that re-establishes percolation. This condition would cause some waste packages to be wetted earlier than others, but the time period for this process to be active is extremely short—only within the first 100 to 200 years after repository closure. After 200 years, some of the waste packages will have cooled to the boiling point of water and the overall re-establishment of percolation will begin. At 1,000 years, most of the repository rock will be below the boiling point of water.

Formation of a precipitation cap was simulated with the near-field model. This model assumed a very restrictive fracture porosity of 0.0001, whereas the fracture testing data indicate a value closer to 0.01. The more realistic porosity would allow some precipitation in the fractures without causing significant closure of the apertures. The reduction of porosity and closure of the fracture openings will also be considered for multiple constituents. These issues will be evaluated in a mountain-scale model to determine if the thermal-hydrologic-chemical (THC) reactions are sufficient to cause a change in the flow paths during and after repository heating.

Comment 12C (page 23): *For these reasons, it is unclear to the Panel that the base case approach of the TSPA-VA correctly captures the behavior of seepage into drifts in the proposed repository and for the unprecedented periods of time considered in the TSPA-VA. Better characterization of the hydrologic properties near the drifts, improved modeling, consideration of coupled effects, and additional experimentation at the drift scale would add confidence to the approach taken. We note that efforts in these directions are currently under way.*

Response: As noted, the M&O is working on refining the analysis of seepage into drifts.

1.5 POTENTIALLY NON-CONSERVATIVE ASPECTS OF THE ANALYSIS

Comment 13 (pages 23–24): *The outcome of the TSPA-VA analysis depends to a considerable extent on the performance of the fuel cladding..., combined with an extended waste package lifetime. Despite the acknowledged corrosion resistance of Zircaloy cladding, this is a remarkably optimistic view of the long-term performance* [for] *this cladding. Zircaloy cladding is typically in the range of 600 to 900 microns thick (less than a millimeter) and, during its life in a reactor, has experienced high temperatures and neutron fluxes. Important changes in mechanical properties can also occur due to thermally induced chemical reactions (oxidation or hydride formation). Another concern is embrittlement.*

To substantiate these comments, the Panel notes the following:

1. *...insufficient information is currently available on stress corrosion cracking.*

Response: The M&O recognized that the model developed for the TSPA-VA (DOE 1998a) was too preliminary and, therefore, it was not included in the analysis. The model for SCC is being enhanced to include both crack initiation and propagation kinetics. In addition, the SCC experimental effort has been greatly expanded and includes an evaluation of crack initiation and growth kinetics under realistic bounding aqueous environments. Further, the potential for reducing residual weld stress is being examined in detail.

2. *...Zircaloy may be susceptible to corrosion under certain chemical conditions ...Additionally, stress corrosion cracking is sensitive to chemical conditions... . These chemical processes were explicitly not considered in the TSPA-VA.*

Response: Local corrosion under extreme chemical environments was modeled in the TSPA-VA (DOE 1998a) by scaling the corrosion rate based on observed zirconium corrosion rates. An improved corrosion model is being developed for zirconium. A better analysis of the chemistry within the waste package is being developed to address both local corrosion and SCC. In addition, the data on SCC tests with various salts that were performed at Teledyne Wah Chang, Albany, Oregon, is being reviewed. Yau has reported no observed SCC in U-bend tests with boiling seawater (Yau 1983) and geothermal salts (Yau 1984). Tests with iodine have shown that SCC occurs at higher stresses than expected under potential repository conditions. Other analysts (Tasooji et al. 1984; Pescatore et al. 1989) have addressed this.

3. *The Panel notes, as it did in its third report, that additional mechanisms of failure remain to be investigated experimentally: (1) pitting and crevice corrosion; (2) hydride-induced embrittlement and cracking; and (3) "unzipping" of cladding due to secondary phase formation particularly uranyl oxy-hydroxides which form immediately as alteration products of UO_2 under moist, oxidizing conditions.*

Response: The M&O has concluded that it is unlikely that pitting and crevice corrosion or hydride-induced embrittlement and cracking will be a major cause of cladding degradation, particularly for waste packages that fail late in life and, hence, only see benign-chemistry water. Work has just been initiated to evaluate the potential for unzipping due either to high-temperature water vapor or to dripping silicate-containing water.

4. *Although the Panel strongly urges that the Project team initiate the necessary experimental programs, we note that time is limited.*

Response: The M&O will utilize the available literature to define the operable mechanisms; however, models will be built upon qualified data. Data that are needed will be developed, although it is recognized that all of the required data may not be available until after the LA. Bounding analyses will be utilized where applicable.

To quote from the TSPA-VA, the "base case cladding model does not have a very wide uncertainty range, so the parameter does not show up in section 4.3 as a top rank-regression parameter." In the Panel's view, this is an instance in which the TSPA-VA analysts have failed to identify the critical importance of a parameter because of optimistic assumptions in the analysis both in terms of performance and the uncertainty in that performance.

Response: Both the ranges and best estimates are currently being reviewed. A sensitivity study for the future LA will look at the absence of cladding.

Comment 14 (pages 24–25): *The analysis of the biosphere dose conversion factors were conducted using the GENII-S model... . This model permits the user to specify the length of time that irrigation waster is deposited on the soil prior to the intake period for which a dose is estimated. In TSPA-VA model runs, this time was assumed to be one year. Taking into account the fact that irrigation in some locations may continue for a period of hundreds or thousands of years, this one year assumption could lead to estimates of radionuclide concentrations in the soil that will significantly underestimate the radionuclide uptake by root crops.*

The degree to which the failure to consider soil buildup leads to an underestimation of the dose rate depends on the specific radionuclides of concern. For technetium and iodine, the default assumption in GENII-S is that these radionuclides are rapidly washed through the soil column. This assumption appears to be inconsistent with measured iodine concentrations in surface soils near release sites for iodine... . Data from these studies indicate that iodine tends to remain in near-surface soils for extended periods. For radionuclides such as neptunium and plutonium, which are readily adsorbed by the soil, the degree to which the dose is underestimated could be significant.

Response: The initial assessment conducted in the TSPA-VA (DOE 1998a) was designed to address the release of radionuclides to the environment over a one-year period in order to be consistent with the regulatory concept of assessing an annual dose resulting from releases in a one-year period. The buildup of radionuclides in soil as a function of previous irrigation activities will be addressed in TSPA-SR/LA. Data on the retention of key radionuclides (e.g., iodine, technetium, and neptunium) will be considered in these analyses.

1.6 POTENTIALLY CONSERVATIVE ASPECTS OF THE ANALYSIS

1.6.1 Transport Through Penetrations in Waste Package

Comment 15 (page 25): *The Panel concluded that the TSPA-VA treatment of the movement of water into a damaged waste package and the transport of radionuclides from such a package were highly conservative.*

Response: The bounding approach was selected because of the uncertainties in the relative locations of package breaches and seeps. The M&O agrees, however, that this approach is conservative for several reasons. The worst pitting is unlikely to occur where the drip is. As the water film spreads over the container, it evaporates, leading to the precipitation of lower solubility materials (silica, calcium carbonate) near the drip and the formation of more soluble, hygroscopic salts (sodium chloride, sodium nitrate) farther from the drip as the last bit of water evaporates. Pitting is most likely to occur near the peak locations for chloride, away from the drip. Drip locations will also move over time. Locations receiving splatter from drips (assuming no backfill) are also more likely to be pit sources. Thus, water is unlikely to initially drip into the pit holes and lead to mass transport. Secondly, if only small amounts of water enter the container, all of the water will evaporate and be unavailable for transport for a significant period of time. Furthermore, leaching and transport from the package cannot begin until the drip rates exceed evaporation. Until then, flow is towards the waste since the waste is the source of heat. In future work, the M&O plans to take credit for evaporation.

Comment 16 (page 25): *As the TSPA staff moves ahead, there is a need for an improved description of the progression of corrosion damage to waste packages, the size and shape of the assumed penetrations, and the distribution of penetrations across the inventory of waste packages. There is also a need for a more realistic conceptual description and treatment of the evolution of corrosion damage.*

Response: The M&O agrees that there is a need to re-evaluate the progression of corrosion damage to waste package barriers. Experimental efforts are underway to assess the likelihood of pitting and crevice corrosion, and the kinetics, under expected aqueous conditions and to better define the expected localized corrosion morphology and progression. In addition, a literature review has been initiated to assess expected SCC morphology and crack-opening displacement based on the SCC experience of the nuclear industry.

Comment 17 (page 25): *Should the corrosion-resistant metals fail by localized corrosion, the likely shapes of the penetrations will be small pits, tight cracks, or narrow channels. The size, shape, and distribution of penetrations in thick layers of corrosion-resistant metals were not analyzed as part of the TSPA-VA; the Panel recommends that this topic be examined in anticipation of the potential LA phase.*

Response: Work is in progress to develop a consistent description for waste package degradation and radionuclide release from the waste package. Additional data and detailed analyses are required to develop: 1) an improved description of the morphology and size of penetrations from individual degradation processes (such as pits, cracks, patch openings, etc.), and 2) temporal and spatial distributions (top, bottom, and side) of the penetrations on individual waste packages. These results, with the information on drift seepage behavior and the interaction of water with the waste form inside a breached waste package, can be used to estimate water ingress and radionuclide release from breached waste packages. The processes or areas that are being considered are: 1) in-drift seepage behavior, 2) water (film) flow on the surface of a degrading waste package, 3) ingress of water into a waste package through the penetration openings, 4) in-waste-package water flow characteristics, mode of water contact with the waste form, and radionuclide mobilization from the waste form, and 5) transport of the radionuclides from the waste package through the penetration openings. The integrated representation of the

above processes in the TSPA analysis will greatly improve the consistency and transparency of the source-term analysis.

Comment 18 (page 26): *Regarding the base case conditions, the TSPA-VA staff assumed that the spent fuel and cladding would be instantly covered by a water film at the time a waste package was penetrated. Transport of moisture and air into the packages and the transport of products from the packages through such penetrations were judged not to provide any significant retardation to radionuclide releases. The Panel does not accept this view; we believe that it would have been more realistic to have assumed that the resulting penetrations will likely retard radionuclide releases from the waste packages. Although the task will be difficult, the Panel recommends that steps be taken to develop better methods for analyzing the movement of radionuclides into and from the waste packages.*

Response: The bounding approach was selected because of large uncertainties associated with the geometry of the system as it evolves over time; however, the M&O plans to make improvements in this area. The M&O is planning a modeling effort to specifically address flow through the drip shields and waste packages to determine if the conservatism in this area can be reduced. Second, the M&O plans to take credit for water evaporation. Leaching can only occur when drip rates exceed evaporation. Until then, aqueous water flow is always towards the waste. Other types of credit are more difficult since it is necessary to know the geometry of failure, which will always be highly uncertain.

If the waste package is breached by small pit perforations or tight cracks that are the likely opening morphology of the waste packages failing initially by localized corrosion and SCC, only small amounts of water could ingress through such openings. This water would be consumed by reactions with the waste package internal materials and the waste form. Some of the water could be retained on the reaction (corrosion) products of those materials and may not be mobile, thus, not contributing to advective transport of radionuclides. The dominant radionuclide release mechanism in such cases would be diffusive transport through relatively stationary water films on reacting materials and corrosion products. The tortuosity of such a transport path would act as a significant barrier to radionuclide release.

Also, see the response to Comment 17.

1.6.2 Retention of Radionuclides in Spent Fuel Alternation Products

Comment 19 (page 26): *At present, the TSPA-VA does not take credit for this type of radionuclide retardation; in this sense, the analysis is conservative. For some radionuclides (^{237}Np and ^{79}Se) some degree of co-precipitation is expected, and for other radionuclides (^{99}Tc and ^{129}I) this type of process is unlikely. For those radionuclides for which this is a likely retardation process, a well-defined experimental program (discussed in section IV.G of this report) may provide a substantive basis for increased retardation of key radionuclides, e.g., ^{237}Np. The inclusion of this type of analysis in the TSPA would, however, increase the general level of complexity of the analysis of spent fuel corrosion and create new data needs which will require further experimental work.*

Response: For the TSPA-93 (Wilson et al. 1994, pp. 9-13), expert judgment was used to define distributions for partition coefficients (K_d's) for a number of elements and materials. The K_d on hematite was evaluated for Np and several other elements. Sorption on hematite is a conservative surrogate of rust since other mineral forms of iron oxide such as amorphous iron oxide and goethite have many more sorptive sites and, thus, higher sorption potential. Sorption of Np on rust from corrosion of the container was used in a Defense Spent Nuclear Fuel (DSNF) Performance Assessment conducted for the National Spent Nuclear Fuel Program (NSNFP) to evaluate the influence that sorption might have on peak release rates. Sorption at the container does delay releases of Np, but only on the order of many thousands of years, not tens of thousands of years (Rechard 1998, pp. 11-26). Hence, not enough decay of Np has occurred to noticeably reduce the peak release. Similar results were observed in preliminary TSPA runs where sorption was included in the UZ and SZ. As a result, sorption at the source term was not included in TSPA-VA (DOE 1998a). Certainly, high sorption will preclude any release of Np in the first 10,000 years; yet Np is not of concern in the first 10,000 years, even without retardation. Furthermore, past analysis for a million-year period indicates that only the time of the peak release can be influenced and that cannot be extended beyond 1 million years.

For TSPA-VA (DOE 1998a), Hardin (1998, Section 6.4.4) reported on sorption experiments using thermally altered concrete to simulate the degradation of the concrete liner. The apparent K_d values were very high. The M&O will consider whether some type of retardation should be included in or around the container in future long-term work.

The retention of radionuclides, particularly ^{237}Np, is currently being examined utilizing spent fuel specimens from the unsaturated drip condition tests. Since concentrations lower than expected were found in the water effluent, it is likely that the Np is being held either in the secondary phases or on metallic surfaces. The effort is focusing on the development of a good mass balance for Np. A companion effort is examining the potential for co-precipitation of Np with uranyl phases.

1.6.3 Potential Sorption of Technetium and Iodine

Comment 20 (page 27): *It seems likely that measurements taken of areas near the Chernobyl site should also provide relevant data on the retention or lack of retention of technetium in the soil. Regarding the retardation of iodine, additional data sets are likely to be available from environmental measurements taken at the Hanford site, where radioactive iodine was released during spent fuel processing.*

Response: The M&O recognizes the need to examine field data from other sites regarding the retention of radionuclides in soils and in the substrate. Information from the literature on Chernobyl is being gathered and will be incorporated into a natural analogue synthesis report. In addition, information from Hanford, the Idaho National Engineering and Environmental Laboratory, Nevada Test Site (NTS), and other sites in the United States will be included in the synthesis report.

Comment 21 (page 27): *Due to the difference between surface soils and the properties of the rock in the unsaturated zone and saturated zone flow paths, the retardation observed at the surface may not occur during underground transport. It is the Panel's view that this question*

should be explored. It is also the Panel's view that the TSPA-VA analysts over-emphasized laboratory K_d measurements and did not appropriately consider opportunities to observe the mobility of radionuclides in the environment.

Response: The M&O also agrees that the retardation of Tc and I needed further study to better understand their potential retardation in the UZ and SZ. Studies of the behavior of I in the environment indicate that organics play a large role in the retardation of this element in surface soils. In addition, SZ retardation/transport of Tc and I appears to be affected by organics (Beasley et al. 1998). Current laboratory studies and results from the German high-level waste (HLW) disposal program indicate that Tc can be reduced by low Eh waters and organics, thus enhancing its retardation. The Eh/pH and organic content studies in the Nye County alluvial system may prove to be very beneficial to the retardation of these elements once they escape the UZ.

There are differences between surface soils and the properties of the rock in the SZ flow paths. The SZ flow and transport model uses retardation factors obtained from the C-well complex tracer tests. A similar complex is planned in the alluvium to conduct tracer and hydraulic tests. These tests will provide data for obtaining the appropriate retardation factors for the saturated flow paths in the alluvium.

The M&O has placed primary emphasis on laboratory measurements of the sorptive properties of aquifer materials for the tuff units. These data were obtained from core samples from the site in both the UZ and the SZ and represent valid site-specific information. In addition, results from the Li-tracer tests at the C-holes confirm that in situ measurements of retardation are roughly consistent with laboratory-scale measurements of K_d's. The C-holes data also suggest that laboratory measurements are generally conservative relative to the tracer test results. Evidence concerning the sorption of Tc from laboratory tests on rocks from Yucca Mountain and on clay materials indicates little or no sorption of this element under oxidizing conditions (Thomas 1987). Iodine is assumed to have no sorption due to its expected aqueous speciation as the negatively charged iodide ion. The assignment of zero K_d to these radionuclides is consistent with values reported in the scientific literature (Brandberg and Skagius 1991). The M&O plans to include a brief analysis of analogue systems with regard to radionuclide sorption and retardation in TSPA-LA.

1.7 POTENTIALLY IMPORTANT BUT OMITTED PROCESSES

Comment 22 (page 27): *For waste package performance, the detrimental effect of the expansion of steel corrosion products on the inner barrier and canister internals has not been addressed.*

Response: A detailed finite-element analysis was performed on the oxidation of the steel outer barrier and the resultant stress to the inner barrier at their interface. However, it was not advanced enough to be included in the TSPA-VA (DOE 1998a). A preliminary result indicated that, at partial wall oxidation, the resultant stress was high but insufficient to damage the inner barrier. However, work in this area was put on hold pending the completion of the LADS process.

Comment 23 (page 28): *Damage due to hydrogen is a major threat to the integrity of zirconium cladding. When cladding is embrittled by hydrogen, it loses its mechanical strength and ductility and fails by through-wall cracks. One possible source of hydrogen in the proposed repository is the corrosion of dissimilar metals in contact with zirconium. Hydrogen formed by the corrosion of steels and stainless steels has damaged and led to failures of zirconium components in industrial applications. If the internal barrier of the waste package is penetrated, water can contact the package internals. The resulting corrosion and hydrogen production represent a significant threat to the integrity of the cladding. This degradation process was not addressed adequately in the TSPA-VA. As a result, the extent of the credit taken for cladding in the analysis is questioned.*

Response: A review of the experiments on embrittlement is in process. Experiments show no tritium gas uptake into the zirconium when tritium was dissolved in water and zirconium oxidation occurred. Other experiments show hydrogen uptake occurs in a reducing environment when the oxide layer can be damaged, but does not occur in an oxidizing environment when the passivation layer is maintained.

Comment 24 (page 28): *Stress corrosion cracking of the C-22 barrier is a realistic threat to waste package performance. The possibility of such a threat was not adequately addressed in the TSPA-VA. A proper evaluation will require more experimental data in realistic, repository environments. The Panel supports the recommendation to use double, U-bend specimens in stress corrosion cracking tests for realistic simulation of repository conditions.*

Response: The M&O has initiated an experimental effort, including the double U-Bend specimen tests, to better understand the conditions under which SCC can occur in Alloy 22 and titanium alloys. The M&O is also initiating an outside literature review to bound the expected waste package residual stress distributions that affect SCC through-wall and lateral propagation. The M&O is also evaluating means to reduce the stress in the highly stressed weld regions utilizing newer techniques such as laser peening.

1.8 DATA NEEDS

Comment 25 (page 28): *The Panel is* [sic] *recognizes that substantial amounts of field and experimental data were developed in support of the TSPA-VA; however, the future success of the Project depends even more critically on the acquisition of additional data, particularly as more sophisticated models are incorporated into the analysis.*

Additional data needs are of two types:

- *Fundamental data that are essential to the development and implementation of the models, and*
- *Data sets designed to challenge conceptual models and test the success of coupled models used in the TSPA-VA.*

Response: During the development of, and subsequent to, TSPA-VA (DOE 1998a), a major focus of the science program has been devoted to acquiring the data needed both to directly support TSPA and to support the natural-system process models that support the TSPA

evaluations. Examples include data being derived from the Nye County EWDP in the SZ down-gradient from the site, field testing at the Busted Butte site, seepage and tracer testing in the Exploratory Studies Facility (ESF), and geochemical sampling in the ESF. Other examples are laboratory experiments on neptunium speciation and solubility and on colloid formation, stability, and sorptive properties.

The M&O believes that the ongoing and currently planned heater tests, as well as analogue studies, will help challenge the conceptual models. The thermal tests are expected to provide additional data that can be used to analyze the capability of the coupled models.

Comment 26 (page 28): *A substantial part of the knowledge base presently rests on expert elicitations ... for data on: flow in the unsaturated zone, the near-field environment, waste package degradation, waste form degradation, radionuclide mobilization and flow/ transport in the saturated zone. Additional site characterization in the unsaturated and saturated zones, as well as experimental programs in waste package and waste form degradation are required.*

Response: The M&O agrees with this comment. As noted in the response to Comment 2, the M&O has ongoing field testing and experimental programs to increase the knowledge base in each of these areas. The M&O is also prioritizing future testing and experimental needs in light of the LADS activity and continued performance assessment analyses.

Comment 27 (page 28): *Solubility limit distributions for the key radionuclides ... have only a limited experimental basis.*

Response: It is true that the current solubility ranges/values for the key radionuclides of interest to performance assessment are lacking or not documented in accordance with quality assurance requirements in the TSPA-VA (DOE 1998a). The M&O is currently conducting literature surveys (including the Nuclear Energy Agency database) and experiments to produce qualified thermodynamic data for the GEMBOCHS (Geologic and Engineering Materials Bibliography of Chemical Species). These data will then be imported into a solubility model (e.g., EQ3/6) to calculate the solubilities of the radionuclides under a wide range of geochemical conditions.

Efforts to produce new thermodynamic data on the key transport radionuclides over the past several years were focused on Np solubility studies, Np co-precipitation experiments, and Tc solubility studies under reducing conditions. In addition to the Nuclear Energy Agency database for uranium, newer literature data are being incorporated into the GEMBOCHS database to help produce a more defensible data set for U.

Comment 28 (page 29): *An experimental program should be developed to advance the spent fuel corrosion model beyond its present empirical representation by a response surface.*

Response: The current approach is considered to be conservative. However, for TSPA-SR/LA, the approach will be reviewed. It is unlikely that new long-term tests will be initiated; however, information from the literature will be utilized for comparison with data generated by the M&O.

Comment 29 (page 29): *There are similar lacks of data for Zircaloy cladding corrosion, secondary phase formation, colloid formation and transport, K_d and saturated zone characteristics.*

Response: The technical basis for cladding corrosion is extensive. Zircaloy degradation for the nuclear industry and zirconium alloy degradation for the chemical industry have been studied for over 40 years. This literature was utilized to determine which degradation modes are likely to be operable under Yucca Mountain conditions. The M&O has concluded that it is unlikely that pitting and crevice corrosion or hydride-induced embrittlement and cracking will be a major cause of cladding degradation, particularly for waste packages that fail late in life and, hence, only see benign-chemistry water. Work has been recently initiated to evaluate the potential for unzipping due either to high-temperature water vapor or to dripping silicate-containing water. Tests that address secondary phase formation and colloid formation and transport are ongoing. These data will provide the basis for the models to be utilized for TSPA-SR/LA.

Our understanding of the generation and stability of colloids formed during spent fuel dissolution is only in its infancy. Current collaborative studies are aimed at determining the stability of the colloids (reverse sorption "K_d" rates) formed during the spent fuel dissolution experiments. These studies will help determine if more information will need to be collected with regards to colloid formation/transport in the near-field environment (NFE).

As stated previously (Comment 5), the Nye County EWDP is expected to provide useful data in what has been identified as a data gap in the southern part of the site-scale SZ flow and transport model domain.

1.9 TESTING MODELS

Comment 30 (page 29): *The Project staff should provide and regulators should require, where possible, demonstrations that the TSPA "works." This can be accomplished by designing experiments and field tests that are driven by the TSPA-VA analysis and that challenge the conceptual models used in the analysis. This is a standard approach in any scientific and engineering study, particularly one as complex as the TSPA.*

An example of such a laboratory study was recently reported by Werme and Spahiu (1998). These authors illustrate the difficulty of modeling actinide concentrations in well-controlled experiments. They conclude, "There is a large body of data on the solubilities of pure actinide phases; however, it appears that the information available is insufficient to explain the experimental results." These conclusions speak directly to the uncertainty in the modeled results in the TSPA-VA. Such experiments cannot be replaced by sensitivity analyses, because the sensitivity analyses used in the TSPA-VA do not directly address the uncertainties associated with the experimental database or the selection of a conceptual model.

Response: The M&O agrees with the importance of demonstrations that the TSPA "works," and that experimental verification is an important part of this demonstration. However, it is not true that modeling analyses cannot be part of it as well. It may be true that the sensitivity analyses in TSPA-VA (DOE 1998a) do not address the kind of uncertainties that are referred to, but sensitivity analyses that do address them could be devised. Furthermore, the kind of system sensitivity analyses conducted for the TSPA-VA (DOE 1998a) can show whether or not more detailed studies are actually needed. If the particular model or parameter is shown not to have much effect on the TSPA results, then a lower level of confidence is acceptable. Also, note that

the probability distributions for uncertain parameters are intended, in part, to address these kinds of issues.

1.10 INSIGHTS FROM THE TSPA-VA

Comment 31 (page 30): *In the TSPA-VA analyses of the performance out to the time of peak doses, typically at several hundred thousand years, almost all of the protection was found to be provided by the engineered waste package, the cladding, and the dilution that occurs in the saturated zone. From this long-term perspective, the early thermal period during which liquid water does not contact the waste packages and the required times for transport of the radionuclides through the unsaturated or saturated zones were found not to be important to overall performance. This has led to criticism that the Project is relying principally on engineered features for protection, and that the natural features of the site contribute little to safety.*

Response: The site is a major component of the waste management system that is intended to isolate radionuclides from the biosphere. The vast majority of radionuclides that provide a potential risk to postclosure health and safety are relatively insoluble or strongly sorbed by the minerals in the host rock, and are naturally inhibited from migrating away from the repository. For these radionuclides, the natural barriers at Yucca Mountain are capable of preventing migration into the ground water. The key aspects of the Yucca Mountain site are a very arid climate, low percolation flux, a thick UZ, and water chemistry that does not mobilize and transport the great majority of the radionuclides.

A small fraction of these radionuclides are potentially mobile or could be transported collodially if exposed to liquid water. For these radionuclides, the engineered barriers are designed to complement the site features. The engineered materials of the waste packages are intended to resist sporadic water contacts for extremely long periods, and the design geometry and components are intended to reduce the amount of water that does contact the waste packages. The combination of natural and engineered features will be required to isolate the radionuclides effectively. Neither type of feature can be or is relied on at the expense of the other.

Comment 32 (page 30): *In the Panel's view, the confidence that the public can have in the TSPA results will, to a large degree, depend on how the analyses of the major attributes of the repository system are conducted and presented.*

Response: The M&O agrees that the method by which the analyses are constructed and presented is critical. In order to communicate the assumptions and the results, it must be possible to see the transparency of the relative contributions of the various components within the context of the total system. The M&O has benefited from the comments and guidance from the Panel, and from other oversight groups, and will continue to address this important issue by improving the clarity and transparency of the TSPA analyses and, also, by using other avenues such as visualization.

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2. THE TSPA-VA METHODOLOGY

2.1 METHODOLOGY

Comment 33 (page 35): *For several of the* [model] *components, however, it is not easy to review or evaluate the degree to which the model abstractions are equivalent to the underlying more complex analyses. For example, the TSPA-VA staff has stated that the modeling of the behavior of the near-field geochemical environment is based on a mixture of "abstracted models with some process level components"... . The document indicates that in at least one area (composition of gas in or around drifts), there is no process-based model. The Panel is unable, based on these comments, to determine what the basis is for the abstracted models. This matter needs to be clarified.*

To help resolve these questions, the Panel recommends that the staff pay careful attention to its own definition of the model abstraction process. In each case, the abstraction should be a simplification of a more fundamental process-based model, and it should provide results consistent with the process-based models over the same range of parameter and input values as can be treated by the more complex process-based model.

Response: The M&O agrees that the process-model basis for all of the abstractions should be clearly defined. This will be addressed in the series of Process Model Reports (PMRs) that will form the basis for the TSPA-SR/LA. Each of these reports will clearly discuss the conceptual and numerical bases for each of the eight component models, along with data used and a comparison of the model results to experiments. Another section of each PMR will discuss TSPA abstractions based on the given component model and how the abstracted model compares with the process model.

Comment 34A (page 35): *The TSPA-VA summarizes the results of extensive sensitivity analyses, conducted for different time periods (typically 10,000, 100,000, and 1,000,000 years), and provides estimates of the effects on isolated subsystems of changes in various performance parameters or site conditions. For example, estimates of the distribution of travel times for radionuclides through the unsaturated zone were based on three different climate regimes. This approach is informative and can provide helpful insights into the likely performance of the proposed repository system.*

The degree to which such analyses reliably indicate which aspects of the system are more or less important is limited by the inconsistent degree of realism versus conservatism in the various analyses incorporated into the TSPA-VA. Because a mixture of both conservative bounding and more-or-less realistic analyses were used, the interpretation of the outcome of the sensitivity analyses is not straightforward. The Panel knows of no methodologically sound approach to quantify sensitivities for a given analysis that uses such an approach. This stems, in part, from the fact that the degree to which the actual performance of some aspect of the repository system differs from an estimate of that performance based on a bounding analysis is not known (if the actual performance were known, a bounding analysis would not be needed).

The Panel's point in noting that the TSPA-VA will inevitably be an uneven mixture of bounding analyses and more realistic assessments is to caution against overconfidence in the validity of

the results of the sensitivity analyses. Because the TSPA-VA incorporated many assumptions of varying validity, the results of these analyses need to be interpreted with judgment and their conditional status recognized.

Response: The M&O agrees that the results of the sensitivity analyses should be interpreted carefully by analysts who are aware of the limitations of the calculations. The fact that a parameter or subsystem has been replaced by some sort of "bounding" estimate can, indeed, affect the results of the ensitivity analysis—not only for that parameter or subsystem, but possibly for others as well. However, the sensitivity analyses are still useful. For one thing, they do indicate the sensitivities of the model system and, therefore, they provide information as to which parts of the model are most important and potentially most in need of improvement.

While problematic for determining "probable behavior," the use of conservative assumptions for some parts of the system is an acceptable approach for showing regulatory compliance, and is even recommended in some areas by the Panel (e.g., for effects of coupled processes).

Comment 34B (pages 35–36): *...the Panel notes that the TSPA-VA staff did not, at this stage, seek to use the sensitivity analyses to demonstrate that certain aspects and/or issues are unimportant and therefore need not be further considered. These judgments and/or decisions may be more appropriately made during the possible TSPA-LA phase.*

Response: The next stage of development of the analyses for the TSPA-SR/LA will focus on developing a prioritization of their importance to system performance, consistent with the evolving postclosure safety case for SR/LA. The prioritization will take into account the NRC Issue Resolution Status Reports for the various components of the TSPA; the comments from the Nuclear Waste Technical Review Board and this Panel will also be considered. The objective of this prioritization will be not only to determine which analyses should not be carried further, but also to determine which elements are most important and, thus, should receive the most attention in the TSPA-SR/LA development.

Comment 35 (page 36): *In its third interim report, the Panel recommended "...that the sensitivity analysis results not be used to identify key analytical uncertainties as the program progresses toward the TSPA-LA. Instead, the Panel recommends that the TSPA sensitivity analyses be viewed as an input to the collective judgment of the TSPA and other project staff. In addition, where sensitivity analyses produce results that are inconsistent with the intuitive judgments of the project staff or advisors, the underlying models and parameters should be examined to ensure that uncertainties in performance are appropriately represented." We continue to endorse this recommendation.*

Response: The M&O is in complete agreement with this comment. It is very important that the analysts continue to question their results in the context of the entire system. The M&O also plans to have the results independently verified and checked by personnel with complementary backgrounds and, thus, expand the intuition and expertise applied to the problem.

Comment 36 (page 37): *...the Panel is concerned that expert elicitation could have been misused by the TSPA-VA staff through its application as a comparatively rapid and inexpensive*

way to synthetically generate "data" as inputs to the TSPA-VA, in place of actual laboratory or field measurements. Unfortunately, in several instances, noted in Section IV, this has occurred.

Response: The M&O structured expert elicitations for the TSPA-VA (DOE 1998a) to be generally consistent with guidance on the use of expert elicitation, such as Kotra et al. (1996) and Budnitz et al. (1997). The goals of these guidance documents are to draw criteria for when expert elicitation should be used from previous expert elicitation projects, both successes and failures, and to define credible procedures for the conduct of elicitations.

Section IV of the Panel's Final Report (Whipple et al. 1999) discusses the use of expert elicitation for the component models for the UZ flow model, waste package degradation, SZ flow and transport, and waste form degradation. The topics covered in these elicitations were identified as significant to the calculated results and were subject to considerable uncertainty. In some cases, data collection activities related to the topics covered in these elicitations provided only a limited basis for quantifying uncertainties, selection among competing conceptual models, and estimating bounds or probability distributions for key parameters. The elicitations were intended to focus on the range of uncertainties that currently exist. By involving experts from outside the M&O who have their own databases and experience, a broader range of perspectives was obtained to support TSPA efforts to characterize uncertainty. In each of these elicitations, the experts were asked for their assessment of data collection or analysis activities that, in their opinion, could lead to a significant reduction in the uncertainties that were assessed. These recommendations will be used to assist in planning additional data collection and analyses to help reduce uncertainties in future iterations of the TSPA process.

If additional expert elicitation projects are planned, the M&O will continue to use existing guidance documents and careful judgment to avoid any unwarranted use of expert elicitation.

2.2 COMPLEXITIES OF THE SYSTEM AND OF ITS COMPONENTS

Comment 37 (page 39): *While the Panel does not think that a fully-coupled, theoretically-defensible, first-principles analysis of coupled processes is possible, it believes that a considerable amount of data exists that could have been incorporated into the modeling approaches used in the TSPA-VA.*

Response: It is true that a considerable amount of data exists and could be used in the determination of phenomena that occur in the UZ above and near the potential repository. Much of the data came from the thermal tests occurring in the ESF. In fact, the temperature results from the Single Heater Test were used by TSPA to perform a series of hydrologic property set comparisons to measured temperature data. With these data, an assessment was made regarding the application of hydrologic property sets for the performance assessment (developed by an ambient model and its governing assumptions) to a thermally perturbed system. Other thermal testing data related to thermal-mechanical and thermal-chemical processes were either just becoming available (as in the case of the Drift-Scale Heater Test) or were not applied due to the large uncertainties associated with a specific (thermal-hydrologic-mechanical or THC) process on affected flow properties. An example of this is the measured rock displacement, which is on the same scale as the Single Heater Test, and how it may be upscaled to a larger scale thermal-hydrological (TH) model with an appropriate constitutive relation governing the fluid

flow. These processes are to be investigated further (with the use of thermal testing data) for the TSPA-SR/LA.

2.3 MANAGING COMPLEXITIES AND COMPONENT MODEL LIMITATIONS

Comment 38 (page 40): *On the basis of its review, the Panel has concluded that there are two types of processes that should be analyzed as part of the possible upcoming TSPA-LA, particularly in terms of meeting the anticipated "reasonable assurance" requirements of the USNRC. These are (1) those for which analytical models are available, and (2) those that may be essentially intractable given current analytical capabilities, or intractable within the time constraints under which the TSPA staff is operating. Although both of these types of processes are complex and extremely difficult to analyze, each has distinct characteristics from the standpoint of the approaches that can be used to analyze them. These approaches include:*

- *Updating the component models*
- *Expanding the quality and quantity of data available as input into these analyses*
- *Use of bounding analyses, that is, intentionally conservative assumptions, parameters, and models*
- *Design changes.*

Also to be considered is the incorporation of the "defense-in-depth" concept into the design of the overall repository system. Effective use of this concept, in concert with the approaches enumerated above, can enhance the confidence of the designers, the analysts, and the regulators that there is reasonable assurance that the proposed repository design will meet the regulatory requirements.

Response: The M&O agrees with the recommended approaches. The M&O intends to identify where the weaknesses lie in terms of being able to evaluate processes in an analytical manner or using some other simplified approach. The effort toward traceability and transparency should further enlighten where such decisions are made. In addition, the M&O and NRC are planning interactions to discuss appropriate defense-in-depth methodologies.

Comment 39 (pages 42–43): *...incorporation of the "defense-in-depth" concept into the design of the overall repository system can also provide increased confidence in the performance of the proposed repository system. ... In nuclear power plant regulation, the objective in applying this philosophy is to assure that the system will perform safely even if one or more individual barriers has failed. The analogous defense-in-depth requirements for a repository are not yet clear. While the assessment of defense-in-depth takes place outside the TSPA and, therefore, outside the Panel's charge, we believe that the TSPA methodology can be a useful tool for assessing defense-in-depth. Just as in the case of the analyses of the performance of nuclear power plants, we believe that the TSPA methodology can provide a means of estimating how well a system of barriers within the proposed repository would perform, even when one or more of the barriers within the system is assumed to have failed... .*

Response: During the LADS process, the M&O started to assess the appropriateness and the methodology for applying TSPA models as a tool for assessing defense-in-depth.

Comment 40 (page 43): *While incremental improvements in the analyses of coupled processes can be made, the Panel has concluded that a detailed, technical defense of these analyses cannot be demonstrated at the present time. As a consequence, the Panel recommends that in the TSPA-LA phase, the processes be treated by the use of either bounding analyses or design changes, supported by the incorporation of the defense-in-depth philosophy into the overall design of the proposed repository system.*

Response: In the LADS process, designs were considered that seek to minimize the effects of coupled processes on repository performance. The reduced importance of these effects would make bounding analyses more feasible and credible. (Bounding analyses are generally nothing more than analyses based on abstracted models.) As such, they are already standard within performance assessment. However, the term "bounding" also generally implies conservatism, which is presumed to require less of a process-model/experimental basis. This is difficult to demonstrate in most cases (especially for nonlinear processes), and in cases where it can be demonstrated, it is only because a very high degree of pessimism has been assumed in the bounding analysis. This sort of pessimism will be avoided wherever possible in the TSPA-SR/LA through comparing the TSPA-SR/LA models against the engineered-barrier system (EBS) 1/4-scale tests, preliminary results of the Drift-Scale Heater Test, and other laboratory experiments and analogues where available.

Comment 41 (page 43): *In the case of thermal-hydrologic-mechanical-chemical coupled processes, the Panel has the following suggestion on how such a bounding analysis could be performed. The suggestion is based on the observation that the output of an ideal analysis of these processes would describe the duration of the thermal period, and the pattern and flow rates of water after the thermal period has ended. Although the Panel does not think that it is possible to analyze these coupled processes in detail, we have concluded that it may be possible to determine reasonable bounds for the following factors. The time curve over which the repository will heat up and then cool. This will enable the analysts to estimate when the waste packages will experience increasing humidity levels, subsequently followed by the flow of liquid water;*

- *The quantity of water that will flow on or into waste packages. This is likely to be bounded by the estimated infiltration rate at the repository horizon for each particular climate regime considered. The infiltration associated with the long-term average climate appears to the Panel to provide a reasonable bounding value.*

- *Where the water will go and how many waste packages will experience liquid drips. The uncertainties in the SEEPS model may be such that the TSPA staff may consider the bounding case in which all the waste packages are assumed to be wet.*

Other effects such as those on the chemistry of the water entering the drifts are likely to be of less importance, because the chemical conditions at the waste package surface are likely to be determined more by the local versus the far-field environment.

Response: The M&O appreciates the Panel's suggestions on developing appropriate bounding analyses. However, in this particular example, alternative designs being considered for SR/LA may limit the need to perform this type of analysis. If the M&O is required to make more detailed models of coupled processes, an approach like this may be useful. However, it must be noted that the range of long-term average infiltration is considered by many reviewers to be unreasonably conservative. Also, allowing all waste packages to be wet at the same time is an extremely improbable assumption, given the volume of water available at one time in the mountain and current knowledge about water flow in this type of unsaturated media. However, it is possible to utilize such a construct in sensitivity studies, as discussed earlier, to help gain a better understanding of the coupled processes.

2.4 OVERALL CONCLUSIONS ABOUT THE TSPA-VA METHODOLOGY

Comment 42 (page 44): *In the course of its review, the Panel has noted the inherent difficulty of several aspects of the performance assessment. Our purpose in doing so is to distinguish between those cases where refinements in the modeling and the acquisition of additional data will permit significant improvements to be made in the analysis, and those cases that may be essentially intractable within the time constraints under which the TSPA staff is operating. Our comments are not meant to excuse the Department of Energy from meeting its obligation of demonstrating with the required degree of confidence that the repository will meet or exceed the specified performance targets, should a license application be submitted the USNRC. Instead, they are to suggest that the approach to resolving deficiencies in the TSPA-VA, and the work toward preparation of the TSPA-LA, should be based on a clear understanding of the nature and cause of each deficiency.*

For cases in which it is feasible to improve either the component models or their underlying data, the Panel recommends that efforts be made to implement such improvements wherever such changes would affect the overall assessment. Where conservative bounding analyses do not result in unduly pessimistic estimates of the total system performance, the Panel recognizes that it may not be cost-effective to spend additional time and effort refining the assessments and making them more realistic. For those issues for which, by virtue of their complexity, it is not feasible to produce more realistic models supported by data, the Panel recommends that a combination of bounding analyses and design changes be applied.

Our purpose in distinguishing between these situations is to acknowledge that there are some aspects of the analysis for which additional data collection and modeling will produce only small reductions in uncertainty. In such cases, we recommend that the TSPA staff demonstrate, where possible, either in the TSPA-VA reference design or in a revised design, that the cited uncertainties have only limited consequences with respect to the overall repository performance.

Response: A major effort is currently underway to identify and address data deficiencies in the TSPA-VA (DOE 1998a). See the responses to Comments 4 and 34B. The path forward for finalizing the process model and abstraction model development will be documented in the PMRs. The PMRs will describe which analyses will be completed and why, which areas will not be pursued and the expected impact, and which data and models would be developed further as construction and performance confirmation proceeds.

The M&O agrees that component models and the underlying data which are determined to be in need of improvement and which affect the overall performance of the system should be updated where feasible. The next iteration of the TSPA will provide updated models and data to the extent that the schedules and resources allow. Additional improvements may fall into the performance confirmation period, post LA. Additionally, the use of reasonable bounding analyses will be included as an approach in the TSPA-SR/LA for addressing certain models and data as appropriate. The SR design that will be selected later this summer will help render the analysis of some of the uncertainties in the system unnecessary.

The TSPA analyses are just one factor in determining whether or not additional data collection and modeling will be conducted. Other factors are considered when determining the potential value and need for additional data collection and modeling. In general, the TSPA analyses attempt to show the very aspect pointed out by the Panel, but these analyses are not the only inputs for the selection of future work.

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3. COMPONENT MODELS OF TSPA-VA

3.1 THE UNSATURATED ZONE UNDER INITIAL CONDITIONS

Comment 43 (page 46): *The accuracy of the current infiltration maps was subject to some criticism by the UZ expert elicitation panel. The validity of future Projections is also questionable, given that they are based on present-day values for the various model parameters (including vegetation, cloudiness, etc.).*

Response: Future climate and infiltration modeling for the PMRs, and the potential SR and LA, will be based on future projections of temperature, precipitation, vegetation, and other aspects. While uncertainty exists, the M&O intends to use a conservative range of infiltration values based on more realistic models of climate and infiltration.

Comment 44 (page 47): *With respect to upscaled flow and capillary properties, the approach taken in the TSPA-VA is to use the van Genuchten model derived for UZ flow in homogeneous soils. Although convenient, use of this model is not justifiable in the present context. Ignored in this approximation are a multitude of processes: the unstable nature of gravity-driven infiltration in real fractures; the possibility of hysteretic (and chaotic) behavior during episodic flow, as documented in recent experiments in related systems (Faybishenko et al., 1998); the effect of sub-grid-scale heterogeneities, including correlated structures, anisotropy in fracture permeability, and saturation gradients; the effect of the connectivity of the fracture and matrix continua; and the effect of abrupt changes in properties on transport fluxes expected along stratigraphic discontinuities. The last item has already been shown to be sensitive to the particular flux-weighting scheme used in the simulations. Also ignored are the differences between wetting and drying cycles, which are expected to develop during the heating period. A similarly questionable approach is used in the modeling of heat pipes in thermal hydrology, where recent findings have shown a complex flow behavior (Hardin and Chestnut, 1997).*

Response: Although approximate, the M&O hopes to capture the global behavior of flow through fractured media with the calibrations and the fact that the models demonstrate a consistency with observed data at the site. The alternatives (e.g., discrete fracture-flow models) suffer similar approximations and assumptions as the dual-continuum models. Discrete fracture-flow models often consider simplified representations of the fractured system, and they usually neglect matrix interaction. In addition, confirmation and testing of these discrete-fracture models would be even more difficult at the scale of the site.

Comment 45 (page 47): *With respect to the representation of the fracture-continuum/ matrix-continuum coupling, the increase in the estimated infiltration rate has forced the introduction in the dual continuum (DKM) model of an adjustable fracture-matrix interaction factor. In this way, a non-trivial fraction of the infiltration is forced to partition in the fracture continuum. Using the inverse modeling calibration procedure, reducing this interaction factor by as much as four orders of magnitude, has enabled the TSPA team to accommodate changes in the revised infiltration rate, without producing unphysical changes in other hydrological properties.*

The introduction of a reduction factor is reasonable and appropriate in order to account for a variety of processes, which are not included currently in the description of physics at the various scales, such as the scale of a single fracture and the scale of a numerical grid block, as mentioned above. However, in the current approach of the TSPA, this reduction factor is simply an adjustable parameter, devoid of convincing physical meaning and often taking values as small as 0.0001. This is not satisfactory and reflects a lack of understanding of the actual physics of the process and, more generally, the lack of progress in the scale-up of two-phase flow in the fractured system, as also noted above.

Response: The fracture/matrix reduction factor has physical meaning. It represents the effects of micro-scale processes such as fingering, coatings, channeling, and film flow. Because it is not possible to fully characterize these processes at the site, the reduction factor is used as a fitting parameter for calibration to the site data. This calibration of the geometric reduction factor was recommended by Gerke and van Genuchten (1993). In addition, the M&O is implementing a new fracture/matrix interaction model that defines the reduction factor as a function of fracture saturation with rigorous derivations of the characteristic curves, based on the effective saturation of active fractures.

Comment 46 (page 48): *The difficulties in the above two issues are compounded by the lack of convincing field data to support the representations taken, inasmuch as reliable flow data have only been gathered from core studies. As a result, the Panel is skeptical of the validity of the base case set of hydrologic parameters and particularly of the van Genuchten-type capillary and flow properties of the fracture network and of the fracture-matrix reduction factor. These are all key variables in the partition of flow between fractures and matrix. Given the significance to other TSPA components (seepage fluxes into drifts, thermohydrology, and UZ transport), the Panel believes that efforts should be made to reduce the existing uncertainties, using analytical studies and field tests. Although acknowledging that the upscaling of UZ flow in a fractured system is a non-trivial task, the Panel believes that such a step is also necessary in order to conclusively and unambiguously determine the relevant hydrologic response of the site in developing the TSPA-VA.*

Response: Although van Genuchten properties are associated with porous media, they have physical meaning for discrete fractures as well. The estimates of hydrologic properties yield results that are consistent with a physically meaningful depiction of the system, thereby furthering M&O efforts to have correlated data. See, also, the response to Comment 47.

Physically, the fracture/matrix reduction factor is a result of sub-grid scale gravitational fingering and coating effects. It should also be noted that although the active fractures correspond to a small portion of the total connected fractures, their number is still very large for a site-scale model. The M&O will provide better documentation of the physical meaning of this factor in the future and develop a two-dimensional (2-D) grid block-scale fracture network model to further explore sub-grid physics. This will provide a means to address issues regarding upscaling, constitutive relations, and confirming continuum approaches for unsaturated flow in fractures. In a dual-continuum approach, fracture flow will occur when the matrix is at less than full saturation.

The M&O agrees with the Panel that better treatment of fracture/matrix interaction is needed to simulate the transport processes more accurately. The decision to use the dual-continuum approaches with a fracture/matrix reduction factor is based on the following considerations:

1. Mathematically, it is not a problem to simulate fracture/matrix interaction more accurately by subdividing the matrix blocks using the TOUGH2 code. However, for a site-scale model, it is not computationally practical.

2. The use of the dual-continuum approach may underestimate the transport into the matrix block. This is because the actual concentration gradients near fracture/matrix interfaces may be larger than those calculated due to the fact that reactions occur near fractures. Since the matrix transport processes correspond to long travel times to the water table, compared to those in fractures, the dual-continuum approach should give conservative predictions of the nuclide transport.

3. In the site-scale model, the M&O does not intend to give predictions of transport at small scales. Instead, the focus is on the large-scale, long-term, overall behavior of the transport processes.

The Panel suggests the use of an analytical solution to deal with transport processes between fractures and matrix. However, the M&O is unaware of an analytical solution for this purpose where the dual-permeability approach is used that is available in the literature. Some solutions exist for matrix diffusion processes under saturated conditions with no advection in the matrix. These solutions would not be applicable to transport between two continua when advection is present in the matrix continuum. Its use would be highly questionable and not defensible.

From an analytical standpoint, the "fracture/matrix coupling factor" used in TSPA-VA (DOE 1998a) is being replaced by an "active fracture" model described by Liu et al. (1998). The authors contend that this approach provides a more defensible representation of flow through a variably saturated fractured rock mass than was previously obtainable through introduction of an ad hoc "fracture/matrix coupling factor." Field tests to further examine this "active fracture" approach are being conducted as part of the seepage tests in the ESF.

The current conceptual model of the UZ flow system considers that the overall behavior of site-scale flow and transport processes are controlled mainly by relatively large-scale heterogeneities associated with the geological structures of the mountain. The complexity of a model incorporating heterogeneity needs to be consistent with the availability of relevant data. This approach is also supported by field observations, such as matrix saturation distributions. For a given geological unit, measured matrix saturation distributions are very similar from different boreholes, indicating that large-scale matrix flow behavior and effective fracture and matrix hydraulic parameters should be similar within the unit. A site-scale model based on a layered approach can be calibrated relatively easily with multiple data sets and would provide a means of incorporating a significant amount of the available site data. It is straightforward to deal with upscaling issues using inverse modeling where a layered approach is employed. This is because effective parameters are inferred directly by matching the large-scale simulation results with grid-scale observations that are averaged from small-scale in situ measurements.

A two-step approach to upscaling is used. Simple averaging schemes are used to estimate block-scale effective parameters and these estimations are then refined, based on inverse modeling. It is important to note that the currently available stochastic theories have been developed for single-continuum systems and, therefore, cannot be directly applied to dual-continuum systems. For example, these theories indicate that large-scale effective permeability can be considerably larger than those at small scales. However, this may not be true for matrices in unsaturated fractured rock due to the fracture/matrix interaction. Large fractures can act as capillary barriers for flow between matrix blocks separated by these fractures, even when the matrix is essentially saturated (capillary pressure is close to the air entry value). Consequently, the presence of fractures may reduce the effective permeability of the matrix continuum.

Comment 47 (page 48): *The Panel believes that at this stage there is still a considerable need for further improvement of the hydrologic characterization of the UZ. This can be obtained by collecting additional data, where possible, by revisiting and relaxing the questionable assumptions made in modeling, and by proceeding with 3-D inverse modeling.*

Response: Additional testing to improve hydrologic characterization of the UZ and to refine conceptual models of fundamental hydrologic process within the UZ, such as fracture/matrix-interaction processes, are ongoing in the North Ramp and Main Drift of the ESF and are planned to be conducted in the EWCD. Testing to collect additional data on the hydrologic and transport properties of the Calico Hills nonwelded unit and to test hypotheses of flow and transport within this unit also is underway at the Busted Butte Field Test site. The problems associated with the simplification of one-dimensional flow in performing the model inversions are recognized, and this restriction is being relaxed; both 2-D and 3-D inversions will be completed to support the future TSPA evaluations.

Comment 48 (page 49): *The Panel believes that the analysis of seepage is an important new contribution. However, because the sensitivity of the seepage estimates depends on the permeability and capillary structure of the fracture continuum in the immediate neighborhood of the drifts, they are subject to the large uncertainty in our knowledge of the heterogeneity, spatial correlation and anisotropy of these properties.*

Response: The Drift Seepage Model will be improved in future efforts. First, the upper model boundary value (determined by site-scale percolation flux) will be revisited, using a more physically based infiltration model. Second, the hydraulic property sets will be recalibrated to recently collected test data from the ESF. This provides hydraulic calibration information to better describe flow at the drift scale and make the model less dependent on small-scale laboratory and site-scale information. Third, additional air permeability information from the ESF will be used to give a better description of the stochastic distribution of the fracture permeabilities. The model will also be revised to consider alternative drift geometries representing partial collapse features. This will simulate asperities along the drift wall that would facilitate a dripping flux. Together, these activities will reduce the uncertainty of the Drift-Scale Model.

Comment 49 (pages 49–50): *Given the importance of seepage, its sensitivity to the flow properties around the drifts, but also the short time that has been available for its study, the*

Panel believes that further work should be done to increase confidence in the TSPA-VA predictions. The following issues require further attention:

1. *Since capillary barriers essentially reflect boundary effects, seepage would be sensitive to the particular geometric and wetting conditions in a small region around the drift wall. The need exists, therefore, for an accurate characterization of the heterogeneity and fracture capillary properties in this area. The effects of the geometrical changes that may result from the collapse of the drift roof in response to thermomechanical or seismic processes need to be analyzed. In addition, given that the actual fracture spacing is of the same order as the grid block size used in the continuum DKM model for the seepage study (grid spacing of 0.5 m), the use of discrete fracture models of transient flow would be more appropriate and should be pursued.*

Response: The model geometry will be revised to consider alternative drift conditions representing partial collapse features. This will simulate asperities along the drift wall that would facilitate a dripping flux. An air gap will be assumed between the drift wall and the waste package. Fracture heterogeneity is included at the drift scale by statistically considering the variations in air permeability.

The current approach is to assume all flow is in the fractures within the dual continuum model. Continuum steady fracture flow is simulated both with homogeneous properties and with stochastic variations in fracture permeability and the van Genuchten alpha. Fractures that drain exclusively into the drifts were also simulated. This work has illustrated that heterogeneity causes a broad range of seepage rates per unit area at low percolation rates (less than 100 mm/yr) and similar seepage rates at higher percolation.

The discrete fracture model could be imposed on two scales. The first scale would be a single fracture extending from surface, through the PTn, and into the drift. This model would examine the maximum effect of transient infiltration bringing water into a drift. The second model would be a discrete fracture model at the drift scale. The test data are currently collected at a 0.3-meter frequency from horizontal bores in the niches. These data could be applied to the inverse method to determine effective fracture characteristics and statistical properties of the fractures. Stochastic flow representations could be compared to heterogeneous DKM modeling to determine the sensitivity of the conceptualization of flow at the drift scale. Discrete fracture modeling will be considered for FY00.

2. *Although recent experimental data are reported to be consistent with the seepage analysis, further testing is needed.*

Response: Ongoing testing in the ESF and new seepage testing to be initiated in the EWCD will extend the knowledge of fracture permeabilities and seepage. A large-scale seepage test is planned between Niche 3 in the ESF Main Drift and the Cross-Over Alcove in the overlying EWCD.

3. *In the TSPA base case, seepage into the drifts is decoupled from TH, and is assumed to only take place following the end of the thermal period and under ambient flow*

conditions. The model also assumes that seep locations and rates are time-independent, under conditions of constant climate, and that the drift geometry remains constant. Many of these assumptions will not be valid.

Response: See the response to Comment 12B.

3.2 THERMOHYDROLOGY

Comment 50 (page 53): *It is important to realize that the process of dissolution is much slower than the process of precipitation, and as a result, a cap of significant thickness is projected to still be present after thousands of years (indicated in Hardin* [1998] *to last as long as 900,000 years). Thus, the properties of the cap in controlling seepage into the EBS, and eventually onto the canisters is of critical importance to the problem of establishing how the environment of the repository will change over time and how this will effect the distribution and quantity of water flowing through the repository.*

Response: Although natural analogues were not specifically mentioned by the Panel as a means of addressing this problem, the M&O will assemble data from geothermal fields that have experienced self-sealing over thousands of years, and will assess the factors that have contributed to the formation of the caps, their longevity, and their effects on permeability of the system over long time frames. This information will be used to help evaluate the conditions under which silica caps would form and remain at Yucca Mountain.

Comment 51 (pages 53–55): *Even though the Panel is unable to determine from the available information whether the results are sufficient to provide the level of information and support needed in the TSPA-VA, the coupled effects and their absence from the TSPA-VA are a significant cause of concern. In the opinion of the Panel, the assumptions made in the TSPA-VA that the effects of THC activities will be short-lived and can be neglected are not warranted... .*

Response: Coupled THC effects in the host rock that may cause changes in the hydrologic conditions that persist beyond the thermal period will be more directly evaluated in the next TSPA using abstracted results of the coupled process-level models. The TSPA-VA (DOE 1998a) analyses attempted to capture some of the transient coupled effects in the models for the gas and water chemistries perturbed by thermal effects, but these were derived only in a loosely coupled way, based on the thermal hydrology process-level model results. The coupled THC models being developed should allow further improvements in the consideration of these processes.

The site-scale UZ flow and transport model has been enhanced to provide the capability of modeling coupled THC effects within the UZ rock mass involving the assemblage of minerals known to be present within the tuff (e.g., silica, feldspar, calcite, zeolites, and clays) in the presence of both water and air, including explicit consideration of the partial pressure of carbon dioxide. This simulation capability will be applied to evaluate the effects of durable changes in both hydrologic and transport properties within the rock mass above and below the repository as a result of chemical reactions induced by repository heat release. This reactive-chemistry modeling capability can be similarly applied at the drift scale to examine near-field effects in the

vicinity of the waste emplacement drifts and is currently being used to predict the expected THC effects in the rock mass affected by the Drift-Scale Heater Test.

Comment 52 (pages 55–57): *...the Panel believes there are some complications in analyzing the thermal processes that need further attention.*

In this regard, the Panel offers the following comments:

1. *The abstraction methodology presented is a commendable attempt to provide answers to a complex problem and represents a significant improvement over the previous TSPA reports. In order to avoid detailed three-dimensional (3-D) thermohydrologic calculations, which are computationally expensive or possibly intractable, the approach taken is to use a quasi two-dimensional (2-D) scheme to analyze TH behavior in drifts in symmetric elements. Variability due to waste-package type, 3-D and mountain-scale considerations are incorporated by conducting less expensive, conduction-only calculations at the mountain-scale. Thermohydrologic and conduction-only models are made compatible by a creative, but heuristic, scheme which maps 3-D conduction-only temperatures to quasi 2-D TH temperatures. Quantities important for other TSPA components, such as temperature, RH and air mass fraction in the drift, are estimated using this approach.*

   In addition to the various problems of modeling the actual physical processes, to which we will refer below, one conceptual problem with such an approach is that detailed information on the temporal and spatial dependence of various properties is sought by using a combination of various approximate methods, which by nature are best suited for estimating average quantities. Another problem is the assumption that the relation between TH properties, such as RH and air mass fraction, and the drift temperature, remain the same as calculated for an isolated symmetric drift, regardless of its environment, the history and sequence of the loading, or the possible lack of symmetry around the drift. As a result, proper account has not been taken of the TH interactions between adjacent drifts and the effects of natural convection. The possibility of heat pipe instability in some locations, with a resulting condensate seepage (as observed in the Large Block Test, Hardin, 1998) cannot be predicted. The method also over predicts the performance of drifts at the repository edge. Coarse scale factors, such as a reduction of the actual heat load to an effective value, are introduced to handle such problems. Although the methodology is a creative approach, it needs to be tested against real data (perhaps in conjunction with the Drift Scale Test) to validate the results of the analyses.

Response: The Panel's comments on the TH abstraction methodology consists of several points: 1) the influence of the assumption of symmetry in the 2-D TH submodels (employed in the abstraction methodology) on the prediction of lateral condensate migration and heat-pipe instabilities, 2) the influence of natural convection, 3) the performance of drifts close to the repository edge, 4) the use of the Drift-Scale Heater Test to validate the abstraction methodology, and 5) the influence of drift-scale variability. The following paragraphs successively address these five points.

The Panel's comment about the abstraction methodology assuming an isolated symmetric drift is partially accurate. The 2-D TH submodels used in the abstraction methodology do not assume that the drifts are isolated from each other. These 2-D TH submodels assume a finite spacing between drifts and are run for a range of thermal-loading conditions spanning those applicable to the edge of the potential repository and those applicable to the potential repository center. However, because the 2-D TH models assume that heating conditions and property distributions are symmetrical about the drift axis, the possibility of a large-scale lateral migration of the condensate (from drift to drift) is not considered in the abstraction methodology. The Panel's concern about the possibility of heat-pipe instability resulting in condensate seepage into drifts was a valid concern for the VA design (DOE 1998b).

The LADS process developed an enhanced design alternative that was specifically designed to prevent the coalescence of the boiling zones between drifts and, thereby, facilitate the drainage of condensate between the drifts. In the enhanced design, preliminary thermal-hydrological calculations indicate that less than approximately 20 percent of the repository horizon reaches the boiling point of water. Because 80 percent of the rock pillar separating drifts never reaches the boiling point of water, it is extremely unlikely that the condensate will migrate laterally from drift to drift. The limited lateral (as well as vertical) extent of the boiling zones also limits the volume of rock in which fractures may undergo substantial changes in porosity and permeability as a result of coupled THC processes. In the VA design (DOE 1998b), the ponding of condensate above the boiling zones was the major factor leading to the development of a very thick heat-pipe zone above the repository horizon. If this enhanced design alternative is selected, it will greatly limit the ponding of condensate above the repository horizon, thereby restricting the vertical extent of the heat-pipe zone to only a few meters.

The Panel's comment about the effects of natural convection being neglected by the abstraction methodology is partially accurate. The effects of thermal buoyancy (i.e., natural convection) are not accounted for at the mountain scale; however, the effects of thermal buoyancy are accounted for at the drift scale. Because the 2-D TH submodels used in the abstraction methodology have lateral no-flow boundaries, and because the water table is a barrier to vapor flow, these models force almost all of the vapor (generated during the boiling period) to flow upward above the repository horizon. This biasing of vapor flow causes almost all of the condensate generation to occur above the repository horizon, thereby over-predicting the condensate drainage flux back into the emplacement drifts. The biasing of vapor and condensate above the repository is equivalent to exaggerating the influence of thermal buoyancy; therefore, the influence of drift-scale thermal buoyancy is over-predicted by the abstraction methodology for TSPA-VA (DOE 1998a). Note that the biasing of vapor and condensate flow only occurs if the boiling zones coalesce between the drifts. For a repository design that does not result in coalescence of the boiling zones, the above-mentioned biasing of vapor and condensate flow does not occur in the drift-scale TH models. For some of the TSPA-SR/LA calculations, the M&O plans to replace the mountain-scale, conduction-only heat-flow model in the abstraction methodology with a mountain-scale TH model and, thus, be able to assess the influence of mountain-scale, buoyant gas-phase convection in the predictions of drift-scale TH conditions.

The Panel's comment about the abstraction methodology over-predicting the performance of drifts at the repository edge is only accurate if the influence of mountain-scale buoyant gas-phase convection is found to be strong enough to significantly enhance the rate of cooling at drift

locations close to the repository edge. Otherwise, the abstraction methodology does not over-predict the performance of drifts (with respect to temperature increase and duration of dry-out zone) at the repository edge. The Panel's comment that the abstraction methodology uses coarse-scale factors to represent the influence of edge cooling at the repository edges is incorrect. The abstraction methodology uses a finely gridded mountain-scale, conduction-only model and functional relations between drift-scale TH models and drift-scale conduction-only models to determine, in a highly resolved manner, the entire spectrum of waste package conditions. These conditions range from the coolest waste package locations on the repository edge to the hottest locations in the center of the repository. Once the abstraction methodology is modified to employ a mountain-scale TH model (rather than a mountain-scale, conduction-only model), the possibility of enhanced cooling by natural convection will be fully addressed.

The Panel's suggestion about testing the abstraction methodology against the Drift-Scale Heater Test is a good idea that can be readily implemented. The M&O plans to use the Drift-Scale Heater Test to test the abstraction methodology. A comparison of the results of the abstraction methodology is planned against a hybrid-scale TH model that nests finely gridded drift-scale models into a mountain-scale model. Recent work has demonstrated that it is computationally feasible to incorporate coupled THC processes into the abstraction methodology. In order to assess the potential importance of coupled thermal-hydrologic-mechanical-chemical processes on drift-scale TH conditions, the M&O plans to incorporate the coupled THC and thermal-hydrologic-mechanical processes into the abstraction methodology.

The Panel's comment that the abstraction methodology utilizes models that are best suited for estimating average conditions is correct in the sense that it predicts local averages throughout the repository area. However, it is important to note that the abstraction methodology does incorporate repository-scale variability of the property and percolation-flux distributions. To address the Panel's comment, it will also be necessary to incorporate the drift-scale variability (i.e., heterogeneity) of property and percolation-flux distributions into the abstraction methodology. Work is underway to include the drift-scale variability of these distributions into the abstraction methodology and to extend the abstraction methodology to predicting the seepage into the drifts during and after the thermal pulse.

2. *As indicated in the discussion on the unsaturated zone flow component, the development of an appropriate method for handling the interaction of fluid flow between fracture and matrix needs further attention.*

Response: The approach used in TSPA-VA (DOE 1998a) to address the fracture/matrix interaction was to use a constant flow factor between the fracture and the matrix; this factor is called FMX, which stands for fracture/matrix connectivity factor. For TSPA-VA (DOE 1998a), the value of the fracture/matrix connectivity factor was on the order of 10^{-4} to 10^{-2} for the repository host-rock units; therefore, the influence of matrix imbibition on the attenuation of non-equilibrium fracture flow was, in effect, assumed to be very small. The very small value of the fracture/matrix connectivity factor may be reasonable for ambient flow in the UZ; however, for TH behavior driven by decay heat from the repository, it probably under-predicts the extent to which matrix imbibition attenuates the fracture flow. The use of a small value for the fracture/matrix connectivity factor is conservative in the sense that it maximizes the tendency for condensate drainage to thwart dry-out and the duration of reduction in the relative humidity.

For TH calculations that account for drift-scale heterogeneity, it also maximizes the tendency for preferential liquid-phase flow (in fractures) to penetrate into the nominal dry-out zone. For TSPA-SR/LA, the M&O plans to incorporate more sophisticated conceptual models for fracture/matrix interaction in the TH submodels employed by the abstraction methodology, such as the active-fracture model (Liu et al. 1998). It will be very important to test the alternative conceptual models for fracture/matrix interaction against the Drift-Scale Heater Test.

3. *Although the effects of thermomechanical interactions have not been included in the TSPA-VA, the Panel believes that they cannot be neglected. The concern of the Panel, in this context, is with the transient variation of the permeability field around the drifts, as a result of thermal effects, which can last for tens of thousands of years, as shown in Figure IV-2. The continuous change of the permeability field will alter the seepage properties in the drifts, as explained in Chapter 2 of the Technical Basis Document. More importantly, these alterations will change, in a currently unspecified way, the location of seeps which will continue to evolve with time. This behavior contradicts the present TSPA-VA scenario, in which seepage is assumed to occur at fixed locations, given a fixed climate... . Whether this effect will be conservative or non-conservative is unclear at this point. Further study is needed.*

Response: It is true that these processes were not considered at the scale of the emplacement drift and their influence on drift seepage properties. A simple sensitivity study (using normal stresses and an assumed constitutive relationship governing aperture and flow property changes) was used to assess thermal-mechanical processes in the flow fields below the potential repository. Work plans have been developed in the TH and coupled-processes workshop for the TSPA-SR that can be used to provide information related to near- and far-field rock property alteration (and its duration) driven by thermal-mechanical processes.

There is currently no basis for simulating a time-dependent weep location. It is unlikely that tests will give us this information in time for the potential SR or LA, so a defensible bounding approach will be used.

4. *In the opinion of the Panel, the nature and continuity of the precipitation cap is a matter of critical importance because the seepage of condensate into the EBS, and the subsequent deterioration that leads to waste package corrosion, will be controlled by the flow properties of the material in the cap ... it is the view of the Panel that this complicated problem of characterizing the parameters of the precipitation cap involves an evaluation of the coupled effects of the THM and THC behavior over tens of thousands of years... . It is suggested that the project staff needs to re-examine this problem to determine if the complicated situation can be analyzed. If not, then an appropriate bounding analysis is needed.*

Response: The capability to model coupled THC effects has been incorporated into the UZ flow and transport model and will be used through numerical simulation to evaluate or bound the expected durable changes induced by repository heat release, such as silica-cap formation, that will affect the hydrologic and transport properties within the UZ. Several different approaches for examining the effects of coupled thermal-hydrologic-mechanical effects are currently being

evaluated, although it is expected that only bounding analyses will be available to support future TSPA evaluations.

5. *Birkholzer and Tsang (1997) have carried out an interesting pretest analysis of the thermohydrological conditions for the DST. They used two-dimensional models to analyze the temporal evolution and spatial variation of the thermohydrological conditions in the rock mass and to evaluate the impact of different input parameters such as heating rates and schedules, and different percolation fluxes at the test horizon. They have also investigated the problem of the fracture/matrix interaction using the limited equivalent-continuum and DKM models. Even so, the Panel is not convinced that the fracture/matrix problem is being properly handled in this work.*

The Panel is of the opinion that the Drift-Scale Test will constitute a major step forward in the process of understanding the complex behavior of the proposed repository under the impact of the thermal field.

Response: As stated in the response to Comment 52B, the active fracture model (Liu et al. 1998), which is a more sophisticated conceptual model, will be used to represent fracture-matrix interactions in the thermal-hydrological simulations for TSPA-SR/LA. The M&O will use information from the Drift Scale Test results to verify the applicability of this model to thermally perturbed flow and transport in the unsaturated zone. This approach is expected to address the fracture-matrix interaction issue satisfactorily.

Observed increases in the permeability of the Single Heater Test block between pre-heating and post-cooling times range from 20 percent to a factor of 3.5. Also, during the heating in the Single Heater Test, permeability decreased by a factor of 2 to 4 in an area outside the dry-out zone, presumably due to the filling of fractures by condensate. Given that the permeability of the repository horizon rocks varies over several orders of magnitude, these relatively limited changes in permeability due to the heating/cooling in the Single Heater Test offer some support to the concept in the TSPA-VA (DOE 1998a) that the changes caused in the hydrologic characteristics of the rock by heat-driven processes are not significant.

The Panel appears to be convinced that episodic seepage of condensate occurred in the Large Block Test. Although Hardin (1998) conveys such an impression, that document was premature in making such a conclusion. One of the two observed events in the Large Block Test leading to this conclusion was directly correlated with heavy precipitation in the area. While precipitation as the cause of the other cannot be ruled out, it cannot be definitely concluded, either.

The Panel is concerned with the formation of silica caps above the emplacement drifts, and the dissolution and precipitation of silica causing changes in the hydrologic characteristics of the rock. Again, although Hardin (1998) and Hardin and Chesnut (1997) convey these notions, it is important to note that these notions are based largely on modeling calculations without much support from observed data. Past modeling calculations showing dissolution and precipitation of silica may have had poorly constrained mineral assemblages and other parameters as input. Also, precipitation of silica has not been observed in any of the thermal tests, except for traces of amorphous silica at two locations in the Single Heater Test.

All three thermal tests (i.e., the Single Heater Test, the Large Block Test, and the Drift-Scale Heater Test) indicate increased wetting below the heated region rather than above it. This phenomenon, predicted by the Dual Continuum Model, is thought to be caused by gravity drainage of condensate via fractures. These observations undermine the notions of condensate cap, ponding, refluxing, and silica caps and, hence, minimizes the uncertainties and adverse impact on performance stemming from such phenomena.

3.3 NEAR-FIELD GEOCHEMICAL ENVIRONMENT

Comment 53 (page 59): *A substantial portion of fundamental scientific work on the relevant geochemical processes and conditions remains to be done. Much of this work is fundamental in that it will provide essential data, determine the efficacy of the conceptual models, and confirm the usefulness of the modeled approach. The Panel emphasizes our concern that this work be completed; however, given the magnitude of the experimental programs required, we suspect that much will still be lacking (particularly experiments with radionuclides and field-scale tests) at the time of the license application.*

Response: The reactive chemistry module that has been incorporated into the site-scale UZ flow and transport model is expected to provide, through numerical simulation, the capability to bound the expected chemical composition of water and gas entering the drifts in the potential repository. See, also, the response to Comment 5.

Comment 54 (page 60): *Although the NFGE models are logically constructed, there is little basis for accepting the results as indicative of repository behavior. The complexity of the models, the large uncertainties in parameter values, and the clearly coupled phenomena suggest that it is unlikely that the present NFGE model captures or usefully portrays the repository conditions in the near-field. Substantial confidence in the modeled results and a significant reduction in uncertainty could be gained from an experimental program designed to test the coupled models and provide essential data. Complex systems, such as the NFGE, cannot be modeled or even constrained with only limited data.*

Response: The reactive-chemistry modeling capability now incorporated into the site-scale UZ flow and transport model will permit the numerical simulation of thermally dependent chemical reactions among aqueous, gaseous, and solid constituents. While considerable uncertainties may attend these reactive-chemistry simulations, they will provide internally consistent quantitative representations of possible chemical processes and conditions, including the dissolution, deposition, and alteration of minerals within the rock mass surrounding the potential repository that will affect the composition of water and gas entering potential waste-emplacement drifts. See, also, the response to Comment 5.

Comment 55 (page 60): *Given this level of complexity, the Project staff should consider the degree to which they can expect to successfully model the near-field environment. We are not recommending sensitivity analysis of the models, but rather a "reality check" of the databases and the usefulness and applicability of the conceptual models. There is considerable experience within the geochemical community in modeling equally complex systems (e.g., geothermal systems, natural analogue studies, studies of trace element behavior in natural systems). The Panel believes that the present NFGE model may well have pushed past reasonable*

expectations of what can be modeled given the present state-of-knowledge. Even if critical parameters were well defined (e.g., in-coming gas and water compositions), it would still be a formidable task to model the NFGE.

Response: The M&O agrees that this is a particularly complex area for modeling to address, and agrees that these models can only represent a first cut at the process of describing the perturbations to the chemistry of this system. However, models of the major changes in the compositional environmental parameters will be needed in order to assess the performance of any potential repository system. The intent of the TSPA-VA (DOE 1998a) models for the near-field geochemical environment (NFGE) in this regard was to take the first step in replacing the previously assumed condition of ambient SZ water chemistry and atmospheric gases with models that utilize all the information that was available to address the major conceptual changes that may occur to the system as it is designed. Although the M&O agrees that this representation is still highly uncertain, it begins to outline the potential conditions that may result, which will help define areas that may be either simplified (because of the inherent uncertainty they bring to the system) or that may be pursued to reduce the uncertainties.

The capability to quantitatively model expected reactive-chemistry processes in the NFE has been enhanced over those available during the development of TSPA-VA (DOE 1998a). The models now available are being tested against field and laboratory data, and will be used to provide quantitative bounds and constraints on the expected chemical composition of the water and gas entering the potential waste-emplacement drifts. The M&O fully recognizes the challenge posed by attempts to quantitatively simulate the complex of reactions involving aqueous, gaseous, and solid-mineral phases in the presence of repository heat release. However, the M&O contends that current capabilities are adequate to sufficiently bound the problem for the purposes of the TSPA evaluations directed towards demonstrating expected repository system behavior with "reasonable assurance."

The Panel has correctly noted that the geochemical literature contains an abundance of modeling studies of natural systems that could be evaluated and applied to bound the M&O's understanding of near-field coupled processes. With respect to thermal coupling to chemical conditions, geothermal systems and hydrothermal ore deposits provide the best potential analogues. These analogues will be evaluated to provide confidence in thermodynamic data for important species, field-measured reaction rates (e.g., New Zealand), identification of important reactions used in models, and which reactions may reach equilibrium, based on field observations.

Comment 56 (page 61): *The Panel notes that even after considerable effort the resulting incomplete description of the NFGE may still contain large uncertainties.*

Response: The M&O agrees that large uncertainties will remain in this area, but in order to develop useful bounds of the possible conditions that the engineered materials would experience, such work is essential. The variety of materials in the drift that depend on chemical conditions is large, so there are numerous compositional information needs in this regard. For example, even if the waste package will perform well within a large range of conditions, there must be a model of the expected conditions to demonstrate that they fall within that range. In addition, the waste form itself may require more stringent constraints. The modeling effort (including data

development) for this area is multi-dimensional and still in its infancy, but some of the major chemical changes can be bounded and utilized as alternate conceptual models within the TSPA. The models should provide the best synthesized understanding of the evolution of the system and be utilized within the limits of their uncertainties.

The M&O fully concurs with the Panel that considerable uncertainties are attached to the attempts to predict quantitatively the effects that may be produced in the NFGE, especially as a consequence of reactive-chemistry processes induced by repository heat release. However, it is the M&O's position that current reactive-chemistry modeling capabilities will allow us to examine the consequences of these processes on radionuclide release and transport from the potential repository in sufficient detail to establish realistic and reasonable bounds on these consequences. It is believed that these bounds will be adequate for evaluating overall repository system performance.

Comment 57 (page 61): *We therefore recommend that the project arrange for a detailed, on-going review of the NFGE and that this review involve the actual use and comparison of modeled results from calculations completed with different geochemical codes and databases followed by explicit confirmation by comparison with experimental results.*

Response: The M&O concurs that there may be value in conducting a review of all of the work being done in the areas of coupled processes and NFE. Prior to LA, a formal peer review of the near-field and coupled-process models, and their supporting data, is being considered as part of the model-validation process.

3.4 WASTE PACKAGE DEGRADATION

Comment 58 (page 62): *Of the specific mechanisms being considered, crevice corrosion appears to the Panel to be the most realistic threat to waste package performance. Therefore, the Panel has concluded that process models and abstractions to determine the likelihood and extent of this type of localized corrosion are an absolute necessity. Because crevice corrosion can occur under environmental conditions that will not sustain pitting, another mode of localized corrosion, concentrating on crevice corrosion is believed to represent a more conservative approach. The TSPA-VA treatment of crevice corrosion was based on the adaptation of a pitting model. While similar chemical and electrochemical processes occur as part of both modes of corrosion, the Panel has concluded that a direct crevice corrosion model would be more realistic.*

Response: The M&O agrees with this comment. The crevice corrosion model used in the TSPA-VA (DOE 1998a) analysis was conservative with regard to the likelihood of crevice formation. The extent and rate of crevice corrosion were necessarily conservative due to the large uncertainties associated with those processes. Spatially, the probability of crevice formation was assumed to be 100 percent for any region of the waste package contacted by dripping water, and it was assumed that crevice corrosion is initiated if a critical temperature threshold is satisfied (crevice solution chemistry was not considered in determining the initiation). The pitting/crevice corrosion rate used was derived from the data obtained from the M&O's Long-Term Corrosion Testing Facility, electrochemical (potentiodynamic) polarization tests, and literature data for aggressive testing conditions containing $FeCl_3$. The use of a direct

crevice corrosion model would be more realistic and could help remove some unrealistically conservative assumptions used in the TSPA-VA (DOE 1998a) analysis. However, given the current state of knowledge, there would be large uncertainties with a direct crevice model, especially in such processes as crevice formation, local corrosion conditions around and inside a crevice, the likelihood of initiation and repassivation of a crevice, and crevice propagation rate. The information and data are being collected; however, they may not be sufficient to adequately evaluate the parameters of such a model. Because of these associated uncertainties and limited information, a simplified model with some conservatism embedded in it may be used again in the TSPA-SR/LA analysis.

Comment 59 (page 63): *As the project staff moves ahead to the anticipated LA phase, there is a need both to improve the models and methods for analyzing water chemistries at the metal surfaces of the waste packages under realistic conditions, and to collect experimental data to validate and verify these models and the associated analytical methods.*

Response: The capability to model reactive chemistry and, thus, coupled THC processes in the rock mass surrounding the potential repository, has been incorporated into the site-scale UZ flow and transport model. This reactive-chemistry module will be used to predict the chemical composition of water entering the waste-emplacement drifts during the thermal pulse. Laboratory plug-flow experiments using columns of crushed tuff over a range of temperatures and water flow rates are being conducted to provide experimental data to test the reactive-chemistry modeling capability. Additionally, the Drift-Scale Heater Test may yield data on water-chemistry changes resulting from chemical interaction with the repository host rock under elevated temperatures.

Comment 60 (page 63): *In the opinion of the Panel, the second most realistic threat to waste package integrity is stress corrosion cracking (SCC). As in the case of analyses of crevice corrosion, additional work will be necessary prior to the possible LA stage.*

Response: See the response to Comment 24.

Comment 61 (page 63): *In the case of the TSPA-VA, the Panel has concluded that fabrication and placement effects on waste packages were not addressed in sufficient depth. Further advances in this area would also contribute to methods for the analyses of juvenile canister failures (those, for example, that have defective welds). One of the conclusions revealed by the TSPA-VA was that juvenile canister failures will dominate the release of radionuclides from the proposed repository during the first 10,000 years.*

Response: The M&O agrees that additional information is required in these areas and is continuing its engineering development activity to obtain the answers needed. Fabrication workshops, performance assessment workshops, and the ongoing development program are conducting tests to evaluate laser peening, different closure methods, and improved nondestructive examination techniques. Areas of local cold work (which can be induced through fabrication, handling and emplacement damage) are being evaluated with respect to localized corrosion, hydrogen uptake, and SCC. Juvenile failures are being reviewed from the data and models that are available and an analysis will be forthcoming this year.

Comment 62 (page 63): *There is also a need for an improved description of the progression of corrosion damage, the morphology of the eventual penetrations, the distribution of penetrations on individual waste packages, and the distribution of penetrations across the inventory of waste packages. In addition, a more realistic conceptual description and treatment of the evolution of corrosion damage is needed.*

Response: The M&O agrees that there is a need to re-evaluate the progression of corrosion damage to waste package barriers and the distribution of penetrations. Experimental efforts are underway or planned to assess hydriding, the likelihood of pitting and crevice corrosion, and the associated kinetics under expected aqueous conditions, and to better define the expected localized corrosion morphology and progression. In addition, a literature review has been initiated to assess expected SCC morphology and crack-opening displacement based on the nuclear industry's SCC experience base. The results will help refine the WAPDEG inputs.

Comment 63 (pages 63–64): *Of increasing interest is the development of a better understanding of the rate of corrosion of steel, and of the generation of thick resistant corrosion products in crevices between steel and corrosion* [resistant] *metals. This is especially true in the case of analyzing the behavior of multi-layer waste packages. The need is to apply these models to the range of scenarios that pertain to the proposed repository.*

Response: The evaluation of the crevice behavior of steel and corrosion-resistant materials (CRMs) is continuing with both long-term corrosion test coupons and galvanic couples. However, the emphasis of crevice corrosion has now been placed on combinations that relate to the alternative designs now under consideration, including couples of Alloy 22, titanium alloys, and Type 316 stainless steel—which are resistant to the formation of thick corrosion products.

Comment 64 (page 64): *In terms of research related to the support of the analyses of waste canister performance, there is a need to determine:*

1. *The realistic, extreme boundaries of water compositions in contact with the waste package surfaces. No rational materials selection can be made without such knowledge. The ensemble of properties and species need to be considered; they should not be evaluated in isolation. For example, dilute chloride solutions can concentrate to a more corrosive solution than would a mixed chloride, sulfate and nitrate solution.*

2. *The lowest temperature at which crevice corrosion can continue (T_{CRIT}). This temperature is a critical factor for materials selection and performance assessment.*

3. *The effects of fabrication, transport and emplacement procedures on waste package performance and specifically on the stress corrosion cracking resistance of metals.*

Response: The M&O agrees that work is needed to address these concerns. See the responses to Comments 8 and 24.

Comment 65 (page 65): *The Panel notes that, at this time, there are insufficient data and analysis to support fully, or to discard any of, the options being considered for a final waste package design.*

Response: Short-term corrosion and electrochemical potential tests as a function of temperature, pH, oxidizing potential, and ionic species are underway and are being augmented by work at outside laboratories. This information will be utilized, along with long-term corrosion data, to develop an understanding of degradation mechanisms and to develop models for localized corrosion. Project data will be supplemented with pertinent data from the literature.

Comment 66 (page 65): *Backfill was not included in the TSPA-VA base case repository design. Although the Project staff attempted to evaluate the wisdom of this decision through sensitivity analysis, the Panel concluded that the effort was inadequate.*

Response: The M&O agrees with the comment. The TSPA-VA (DOE 1998a) analysis for the backfill (crushed tuff) effects was limited due to a lack of relevant data. The exposure condition parameters of the outer barrier (carbon steel) corrosion degradation model are temperature and relative humidity. Many important effects of backfill would exceed the currently predicted perturbations to the temperature and relative humidity in the emplacement drifts. Backfill could potentially affect in-drift seepage flow, bulk water chemistry, local water chemistry on the waste package and at the contacts of the backfill particles with the waste package, etc. Additional data and detailed analysis are required to properly address the backfill effect on waste package degradation under the potential repository conditions.

Comment 67 (pages 65–66): *Backfill can also influence the flow of moisture to waste packages and the transport of radionuclides from those that are damaged. Every effort should be made to understand its impacts in anticipation of the LA phase and the accompanying need to evaluate various design alternatives.*

Response: Models and bench and field-scale experiments are being used to further improve the M&O's ability to predict the long-term performance of backfill from THC perspectives. Backfill is recommended as an option for further study by the LADS process. It has potential value as a means of protecting the waste packages and drip shields from rockfall, to eliminate the need to predict rockfall size and timing, and to avoid the crevice and pitting corrosion windows of susceptibility.

Comment 68 (page 66): *The previously cited expansion of steel corrosion products is another issue to be addressed. The analyzability of backfill and drip shield design alternatives will be a continuing issue as the TSPA staff approaches a possible LA phase.*

Response: The use of backfill to reduce the contact of water with the waste packages would be beneficial, if successful. Other design alternatives considered by the TSPA-VA (DOE 1998a) staff included both capillary barriers and drip shields. With capillary barriers, the concerns are emplacement control, long-term stability, settling, and movement. Designs and concerns related to drip shields include: 1) a monolithic canopy, long-term stability; 2) a ceramic coating, application and adhesion; and 3) a thin outer layer of Ti or C-22, fabrication and durability.

Also, see the response to Comment 22.

As stated in a preceding response, the M&O is using models and experiments to improve the analysis of backfill. For drip shields, the LADS process evaluated a 2-cm-thick Ti drip shield with overlapping segments as a placeholder for a drip shield design. The M&O may pursue that

design during the time leading up to the potential SR/LA. The three options and potential failure modes listed by the Panel are potential candidates for the design and its analysis.

Comment 69 (page 66): *There are important linkages among time, temperature, wetness and chemistry. For this reason, there is a need to focus on those parameters that determine waste package performance and to identify and clarify the linkages between the input needs of the corrosion process models and the experimental data being generated. The Panel recommends that more attention be focused on possible combinations of the conditions that may pertain.*

Response: The M&O agrees that this work is needed. An effort is currently underway to evaluate the chemistry and boiling point of saturated J-13 salt that has precipitated on the metallic substrate as a result of evaporation under high relative humidity conditions that promote the formation of water films. A parallel effort is underway to calculate the chemistry utilizing the EQ3/6 code; it is realized, however, that even with Pitzer's corrections, the analysis breaks down near saturation. When this work is concluded, the M&O will determine what additional tests are required to understand the impacts on corrosion behavior. See, also, the response to Comment 8.

Comment 70 (page 67): *At the present time, the corrosion behavior of the waste packages with backfill or rock debris covering the waste packages is not well defined.*

Response: The M&O is evaluating these conditions from a variety of perspectives. First, there are corrosion tests underway in the Long-Term Corrosion Test Facility utilizing groundwater that has been modified by contact with concrete. Second, the M&O has had corrosion couples in the Large Block Test that are currently being removed for analysis. Specimens have also been inserted into the Drift-Scale Heater Test. Laboratory tests in the relative humidity chambers will be initiated shortly that include the dripping of J-13 waters onto heated coupons. Some of these tests will include crushed rock along with precipitated salts.

Comment 71 (page 67): *Radiolysis can generate more oxidizing species in the waters and increase the Eh of the solution. For the base case waste package design, which includes thick steel packages, the TSPA-VA staff concluded that radiolysis does not have a significant effect on either solution chemistry or corrosion behavior. The Panel recommends that this conclusion be documented.*

Response: The M&O agrees with this comment. Documentation of this conclusion is ongoing.

Comment 72 (page 67): *The Panel recognizes that the treatment of MIC degradation of waste packages is uncertain. Nonetheless, there has been no documentation that MIC is likely to shift the waste package environments beyond the range of uncertainty that already exists. This is especially true in the case of steel. In conducting the sensitivity study for the effects of MIC on this metal... the TSPA-VA staff assigned a multiplying factor of five to the corrosion rates. On the basis of its review, the Panel has concluded that this approach is highly conservative. With respect to CRM corrosion, some experts have concluded that MIC is unlikely to affect the corrosion of CRM in any significant manner... . The Project staff has provided no documentation that MIC will increase CRM corrosion rates beyond the current range of uncertainty.*

Response: The M&O agrees that the evidence to date has not shown microbiological corrosion effects in CRMs. However, testing is underway in microcosm experiments and in relative humidity chambers to confirm the expected behavior of these materials. In addition, samples have been exposed in the Large Block Test and are being recovered for examination, and other samples are being exposed in the Drift-Scale Heater Test. These samples are open to the environment in the heater tests and may be assumed to allow for microbiological corrosion, if it occurs.

Comment 73 (page 68): *A detailed review of the WAPDEG model, and the many supporting process models, was beyond the scope of the Panel. Because of the importance of this subject, however, the Panel recommends that the model parameters, underlying assumptions, associated justifications for the treatment of certain conditions, and a comparison of this model with alternate treatments, be subjected to a detailed critical review.*

While the WAPDEG model was useful in providing improved understanding of the corrosion behavior of waste packages for purposes of the TSPA-VA, the Panel concluded that a significant rework of the waste package degradation model will be necessary for the possible LA phase... . While it is rational, the WAPDEG treatment is not unique and alternative approaches should be reviewed and the results compared and contrasted. The Panel recommends that this be done.

Response: The model parameters, underlying assumptions, and associated justifications for the treatment of certain conditions that were employed in the TSPA-VA (DOE 1998a) analysis were documented in a number of analysis documents. Those analysis documents are cited in the TSPA-VA TBD (CRWMS M&O 1998). The WAPDEG code used in the TSPA-VA (DOE 1998a) analysis was baselined. In the process of baselining the code, the WAPDEG model predictions were compared with hand-calculated results for simple cases.

The SR/LA version of the WAPDEG model, currently undergoing an extensive modification, is designed to be flexible to analyze alternative conceptual models, and waste package and EBS designs. The SR/LA version will include additional important waste package degradation modes of candidate materials such as SCC and hydrogen-induced cracking (for the Ti barrier). Extensive documentation, verification, and validation exercises are currently underway as part of the quality assurance process for the potential SR/LA. In addition, the process-level information and models, and their abstractions that will be implemented in the revised and updated WAPDEG model, will be reviewed in detail. To the extent possible, the WAPDEG model and its results will be compared with those from sources external to the Project.

Comment 74 (page 70): *The waste package is assumed to be breached when both barriers are estimated to have been penetrated by corrosion. The Panel concludes that this treatment is logical; however, major information needs remain, especially in anticipation of the possible LA phase. ...In order to increase confidence and transparency, the Panel recommends that the model be applied to a simplified case, e.g., a single patch, and that the evolution of corrosion damage with time be described. It would be useful if estimates covering the realistic range of anticipated environmental conditions (severe, moderate, and benign) could also be provided.*

The Panel also concluded that, in terms of the WAPDEG model, a more rational and stronger case needs to be made for the linkage between the process models and the abstractions

developed for analyzing localized corrosion. There is a large number of process models that deal with a number of degradation modes or engineering enhancements. The overall story or rationale for how these fit together and lead to the determination of waste package degradation was not clearly developed within the TSPA-VA. Further development would aid credibility and also lead to a better definition of data needs and linkages to the process models.

Response: The WAPDEG model was developed and continues to be updated with the following objectives: 1) to bring a more realistic analysis of waste package degradation in the potential repository (rather than taking a very conservative approach, which is routinely done to simplify the analysis); 2) to capture the effects of variation and uncertainty both in exposure conditions and degradation processes over a geological time scale; and 3) to perform analysis within a reasonable computational time and resources. The WAPDEG model has adopted a stochastic approach to achieve the above objectives. To provide the user with reasonable flexibility in conducting analysis under the potential repository conditions, the model has evolved into a large, complex simulation code. The current model also has features for analyzing deterministic cases by supplying appropriate input values and switches. As the Panel has suggested, the current model can be used to analyze the degradation of a single patch or a single waste package with appropriate input parameter values. Although no analyses for deterministic cases were documented in the TSPA-VA TBD (CRWMS M&O 1998), some of these features were used in a process to baseline the code, where simple deterministic case results were compared with the hand calculations.

Efforts are being made for the SR/LA version to improve the model for an enhanced capability to conduct analyses for deterministic cases. This would make the model validation easier and improve the transparency of the model. As discussed in responses to the Panel's other comments, the individual corrosion models and parameters in the current WAPDEG model will be updated and improved as part of the improvement of the SR/LA version of the model by incorporating additional data and analyses. Additional important corrosion modes and their models (such as SCC) will also be incorporated. Abstractions of the process-level models will be developed so that important features of the process-level models are captured as explicitly as possible, and that the degradation processes and their characteristics are properly represented in the waste package degradation analysis.

Comment 75 (pages 70–72): *Because of a lack of data for the various input parameters, the TSPA-VA staff depended to a large extent on expert elicitation. The Panel highlights this dependency on expert elicitation in Table IV-5, where the parameters and models based upon expert elicitation are identified. While these estimates were useful for the TSPA-VA, the Panel concluded that significant improvements in the information base will be required in preparing the anticipated TSPA-LA.*

Response: The M&O agrees with this comment. Additional data and detailed analyses are required to develop the information base that is needed to update and improve those corrosion models and parameters that were developed from the expert elicitation in TSPA-VA (DOE 1998a).

Comment 76 (page 72): *The primary outputs of the WAPDEG model are the estimated corrosion penetration behaviors for a wetted and non-wetted package. The results are applied*

to the estimated fraction of the wetted and non-wetted packages in each region of the proposed repository. The Panel believes that this approach is too limited. Further consideration and analysis is required for the case of canisters made of C-22 that are exposed to moist sand and covered by thick layers of corrosion products. This is the likely exposure condition for waste packages after deposits or debris accumulate on the surface, corrosion products build up on the metal surfaces, or backfill is placed over the packages. The presence of saturated or unsaturated particulate matter will affect the environmental conditions at the metal surface and will also affect the corrosion process through the control of water transport to and from the metal surfaces. The TSPA-VA staff did not address this issue through either expert elicitation or experimentation.

Response: In the TSPA-VA (DOE 1998a) analysis, one major parameter in determining the corrosion mode(s) of the Alloy 22 inner barrier was the presence or absence of water dripping on the waste package. Under dripping conditions, a critical threshold temperature was used to initiate localized (crevice and pitting) corrosion. As the above comments point out, the effects of deposits or debris accumulation, corrosion product buildup, and contact with rock rubble on the inner barrier corrosion were not addressed explicitly in the TSPA-VA (DOE 1998a) analysis. However, attempts were made to capture those effects in the analysis with some conservative assumptions. The M&O assumed 100 percent probability of crevice formation on the CRM inner barrier patch underneath a breached corrosion-allowance material (CAM) patch to represent the effect of those conditions indicated in the comments above. The potential effects of those conditions on corrosion rates were not addressed in an explicit manner. An attempt was made to capture those effects indirectly by sampling the corrosion rates over a given range.

Comment 77 (page 72): *Inputs for the models used in the TSPA-VA to analyze the corrosion of carbon steel, the associated corrosion rates, and other information needs, were based on expert elicitation. While the results are useful and valid for a conceptual understanding, the Panel concluded that further analysis will be required for the LA phase. One aspect of the treatment that the Panel believes is overly conservative is the assumed significant increase in pitting in the presence of alkaline solutions (pH > 10). This behavior has been broadly accepted by the TSPA-VA staff and has led to considerations for restrictions on the use of concrete in the engineered barrier system. Based on the potential impacts on design considerations, the Panel believes that this topic is worthy of further analysis and experimentation.*

Response: The M&O agrees that the initial treatment was somewhat conservative. Data collected to date from the Long-Term Corrosion Test Facility do not show any localized attack (i.e., pitting) as a result of exposure to high pH concentrated J-13 water or to concrete-modified water. It is believed that this is due to the presence of buffering species in the water; however, the design change was not driven by this aspect of corrosion. Rather, it was likely driven by the influence of the high alkalinity on the potential for enhanced radionuclide release. Since the LA design is unlikely to contain large quantities of concrete, additional analysis and experimentation to address the Panel's concern may not be necessary.

Comment 78 (page 73): *On the basis of its review, the Panel concluded that a waste package design with an inner layer of steel and an outer layer of corrosion resistant metal cannot be analyzed adequately using the version of the WAPDEG model that was applied in the TSPA-VA. The likely penetration shape for a CRM/steel scenario is a small pit or a tight crack through the*

corrosion resistant metal, which then exposes the underlying steel. The transport of moisture and oxygen through the penetration will control the corrosion rate. While more detailed analysis is required, it is likely that the corrosion rate will decrease significantly with time. The comparable corrosion rates applied to a steel outer barrier in the TSPA-VA are too high for the restricted geometry conditions of a tight crack or pit in the CRM with exposure of the underlying steel.

Response: The M&O agrees that the current WAPDEG version has a limitation on explicitly analyzing the performance of the CRM-over-CAM waste package design. However, the current WAPDEG version has a feature that allows the user to assign an adjustment factor for the general corrosion rate of the barriers to be modeled. The adjustment factor for the general corrosion rate can be a single fixed value or a distribution. In a WAPDEG analysis, the general corrosion rate from the corrosion model is adjusted by multiplying the rate by the adjustment factor. If the corrosion rate reduction factor is known for the CAM inner barrier underneath a crack or pit opening of the CRM outer barrier caused by localized corrosion, such a reduction factor can be used to capture the decreased corrosion rates of the underlying CAM barrier. However, this is not an explicit representation of such corrosion degradation processes. The SR/LA version of the WAPDEG model will have an enhanced capability to analyze waste package degradation processes in more explicit ways with additional details, and also a greater flexibility in analyzing alternative waste package and EBS designs.

Comment 79 (page 73): *To evaluate the effects of key uncertainties and specific issues on repository performance, the TSPA-VA staff performed several sensitivity studies relevant to the waste packages... . The Panel concluded that these analyses were useful and provided a better understanding both of how the repository performs and of how the TSPA-VA staff attempted to capture this performance using realistic models and evaluations. The Panel recommends that these results be recognized as works in progress that provide useful insight; however, the quantitative results should be viewed with caution... .*

The impact of the general corrosion rate of C-22 under dripping conditions is evaluated in a sensitivity case within the TSPA-VA packages... . The results lead to three important Panel observations: (1) there are insufficient data on the corrosion rates of C-22, (2) there is insufficient information on the realistic environments that will be present immediately adjacent to the waste package surfaces and (3) these data are necessary for estimating potentially important effects on the performance of the proposed repository. The corrosion rates for C-22 recommended by the expert... and used in the TSPA-VA vary over five orders of magnitude. The Panel concludes that the treatment of C-22 corrosion rates and the allocation of total variance to their variability and uncertainty need to be improved prior to the anticipated LA phase.

Response: The M&O agrees that the results of the waste-package-degradation sensitivity analysis in the TSPA-VA (DOE 1998a) are works in progress, and that the quantitative results should be viewed with caution. The M&O also agrees that the WAPDEG model needs a more realistic representation of local exposure conditions on the waste package surface (especially for the Alloy 22 barrier), the corresponding corrosion modes, and their penetration rates. One of the major efforts that is underway for the SR/LA analysis is to develop a more defensible approach to representing uncertainty and variability of the waste package degradation under the potential repository conditions. An enhanced understanding and quantification of local corrosion

conditions on the waste package will help reduce uncertainty in the waste package degradation analysis and increase the defensibility of the analysis results.

Comment 80 (pages 73–74): *Two sensitivity cases analyzed in the TSPA-VA dealt with the moisture flow by drips... and the pattern of seepage into the drifts... . The latter deals with the percentage of the waste package surface area that is wetted as a function of time. The results of both cases emphasize the important impact that these two factors have on the performance of the proposed repository. The Panel agrees with the TSPA-VA staff conclusion that a variety of different alternative models might be imagined for these processes. These results support the Panel conclusion that it is prudent to design waste packages for wet conditions. The higher the confidence that the waste packages will remain passive and have low corrosion rates even when wetted, the more credible it is that realistic times to penetration will be many thousands of years into the future.*

Response: The M&O is re-evaluating its position regarding the fraction of waste packages that experience water. From the materials testing perspective, however, wet conditions have always been assumed. For this reason, the Long-Term Corrosion Test Facility was set up to evaluate the corrosion performance of the candidate materials under a variety of aqueous conditions.

Comment 81 (page 74): *Two sensitivity cases in the TSPA-VA dealt with processes that can change the composition of waters in contact with the waste packages. One was the interaction of seepage water with concrete in the drift liner...; the other was the presumed impact of microbial activity, which can lead to changes in water chemistries and possibly increased rates of corrosion... . The Panel recommends that the conclusions of the TSPA-VA staff in both of these areas be reassessed.*

As recognized by the Project staff, the pitting model for steel may be unrealistically conservative. The presumed behavior is that an increase above 10 in the pH of the contacting waters, due to the presence of concrete, will lead to the initiation of a pit growth process. This, in turn, will lead to a significant increase in the penetration rate of steel canisters. Acceptance of this as a real, detrimental process has led to discussions on the possible need to limit the use of concrete in alternate design).... The Panel does not agree and recommends that this situation be reviewed and re assessed.

In a similar manner, the Panel does not accept the conclusion of the TSPA-VA analysts that MIC has a significant, detrimental effect on the performance of the waste packages and the proposed repository. The outcome of the sensitivity analysis, on which this conclusion was based, was due primarily to the assignment by the TSPA-VA staff of an "enhancement factor" that led to an increase in the presumed corrosion rate of carbon steel. Following this approach, the corrosion rates for the base case were increased by a factor of up to five. This led to a much more rapid penetration of the outer steel layer. The Panel concluded that, given the range of values and the uncertainty of the corrosion rates used in the base case of the TSPA-VA, the assignment of an "enhancement factor" for MIC is likely to be unrealistically conservative.

The Panel recommends that the generalization of the conclusions regarding the effects of high-pH waters and MIC should be avoided, because both processes are analyzed exclusively with respect to the potential impacts on the corrosion rates of carbon steel. Neither process has

been shown to have an impact on the corrosion rates for corrosion resistant metal. The detrimental impact will be highest for the base case canister design with an outer barrier of carbon steel. It will likely have less or no impact on a canister design with an inner steel barrier, and it will likely have no effect on a canister design with all CRM barriers.

Response: Sensitivity analysis results for the effects of concrete-generated high pH water and microbiologically induced corrosion of the carbon steel outer barrier were presented in the TSPA-VA TBD (CRWMS M&O 1998). These results were presented with the caveats that the process-level information used in the analyses was preliminary and needed further analysis and testing, especially the high-aspect ratio pitting model of carbon steel derived from expert elicitation, which is not supported by the site-specific data from the Long-Term Corrosion Testing Facility. The M&O agrees that the effect of the two processes (high pH water and microbiological corrosion) will be much less (or probably of no effect) for waste package design with Alloy 22 as an outer barrier. This concept has been recommended in the LADS effort.

Comment 82 (pages 74–76): *...the Panel identified physical events and processes that have a potential for effects on the waste packages but were not considered, or not sufficiently covered, within the TSPA-VA. These events and processes are itemized here, and all are deemed by the Panel to be crucial to the determination of waste package performance.*

1. *Expansion due to the formation of iron oxide corrosion products...*

Response: See the response to Comment 22.

2. *Insufficient treatment of fabrication and placement effects.*

Response: See the response to Comment 61.

3. *Corrosion processes in moist sand/particulate matter. After an initial period, waste packages are likely to be covered with particulate matter rather than exposed with clean metal surfaces. The potential impacts of these conditions on corrosion rates have not been analyzed or experimentally evaluated.*

   For a steel outer barrier, the Panel concludes that the corrosion rates used in TSPA-VA were non-conservative for the condition of moist sand and particulate matter... . In the case for a canister with a CRM outer barrier, the Panel concluded that the effects of moist sand and particulate matter against the metal surface were neither studied nor certain.

Response: See the response to Comment 70. The M&O also agrees that sand or particulate matter could increase the corrosion rate of a steel outer barrier. At the time of the TSPA-VA (DOE 1998a), this condition was not evaluated, however, testing to evaluate this condition is currently underway. In addition, the M&O is evaluating several alternative designs that do not employ a steel outer barrier.

4. *Corrosion of steel beneath the CRM.... The transport of moisture and oxygen through the penetration will control the corrosion rate which, for steel as noted above, is much lower under conditions of restricted oxygen transport than for surfaces that are freely*

exposed. While more detailed analysis is required, it is likely that the corrosion rate would decrease significantly with time.

Response: The M&O agrees that the rate of corrosion of steel inner barriers would be significantly less than the rate utilized for steel outer barriers. The M&O is considering a reverse VA design (DOE 1998b) that would have a CRM outer barrier over a steel inner barrier. However, the inner barrier corrosion may still be influenced by oxide wedging or other localized process that would mechanically degrade the outer barrier. Hence, the M&O is also considering the use of an inner stainless steel barrier, which will be less susceptible to these mechanisms.

5. *Incomplete status of the analysis of stress corrosion cracking of C-22 and other Ni-Cr-Mo alloys.*

Response: See the response to Comment 13.1

Comment 83 (pages 76–77): *The Panel concluded that the experimental data available to the TSPA analyst were insufficient for determining (a) the performance of various alloys under anticipated conditions within the repository, and (b) the composition of the water that will interact with the waste packages. Many thermodynamic data and kinetic rate constants are unknown or uncertain. Experimental data are required to verify and validate the analytical models. Some important areas of need are presented below:*

1. *Determination of a realistic range of waters that might contact the waste package metals. No rational materials selection can be made without knowledge of the characteristics of the waters in contact with the waste packages.*

Response: See the response to Comment 8.

2. *Establishment of realistic extreme boundaries of water compositions in contact with the waste package surfaces. To accomplish this goal, the combinations of pH, Eh, Cl, NO_3, SO_4, CO_3, Fe^{+++}, Ca, Mg, and so forth, need to be determined experimentally. The results can then be used to validate and verify the models of water chemistry.*

Response: See the response to Comment 8.

3. *Estimation of the temperature where waste packages become wet (T_{WET}). The waste package surface will be dry when it is above this temperature, and corrosion rates will be extremely slow. An increased concentration of ionic species in the water, capillary action from particulate matter on the surface, surface roughness, and the presence of crevices will increase the critical temperature. The values of T_{WET} for the formation of a moisture film on waste package surfaces under realistic conditions need to be determined.*

Response: The M&O agrees that this work is needed. See the response to Comment 69.

4. *Determination of the lowest temperature which crevice corrosion can continue (T_{CREV})... . The Panel recommends that such alloys as 316L, 825, 625/C-276 be*

included in the corrosion tests to determine a multiplying factor or level of comfort for the more resistant C-22.

Response: See the response to Comment 64. The M&O has these alloys under test in the Long-Term Corrosion Test Facility. In addition, some of these materials are utilized in short-term tests to obtain baselines for the more CRMs.

5. *Determination of the corrosion resistance of titanium....The Panel recommends that the likelihood of corrosion due to fluoride be evaluated.*

Response: The testing of titanium alloys is being evaluated in the Long-Term Corrosion Test Facility under a variety of conditions from acidic (pH 2.7) to basic (pH 10) with both dilute and concentrated J-13 groundwater. Some specimens have achieved two years of exposure and will be examined shortly. In addition, short-term tests under electrochemical potentials have been performed. Other tests are planned to evaluate hydrogen embrittlement.

The corrosion resistance tests of titanium alloys in the presence of fluoride are being conducted under the same conditions. For the concentrated J-13 solution, the fluoride content has increased by roughly one thousand times. The fluoride effect is being evaluated in the presence of other ionic species.

6. *Clarification of the corrosion penetration rate and morphology of attack for metals in the passive state for long periods of time (thousands of years).*

Response: The M&O recognizes that for many of the CRMs being considered, the corrosion resistance relies on the long-term integrity of the passive film. The character of the passive film is being studied for materials exposed in the Long-Term Corrosion Test Facility and for materials exposed under short-term aggressive conditions, usually utilizing electrochemical polarization. The principal method of evaluation is the atomic force microscope, but other techniques are also being utilized. The combination of long-term and short-term tests should provide the information needed to understand the morphology of attack and to develop models that predict the corrosion rate.

7. *Determination of the stress corrosion cracking resistance of C-22. The Panel recommends that corrosion studies of C-22 include the addition of double-U-bend specimens and the measurement of crack growth rates for pre-cracked specimens.*

Response: See the response to Comment 24.

8. *Elucidation of the effects of fabrication and emplacement on waste package performance.*

Response: See the response to Comment 61.

9. *Conduct of short term corrosion and electrochemical tests.*

Response: See the response to Comment 65.

10. Evaluation of the effects of thiosulfate and other reduced sulfur species.

Response: The M&O recognizes the need to conduct this evaluation. It has already initiated studies of thiosulfate in its microbiological corrosion activity, with an emphasis on nickel alloys. In addition, a detailed experimental evaluation of the effects of thiosulfate and other reduced sulfur species on localized corrosion susceptibility has been proposed.

Comment 84 (pages 77–78): *As a final comment, the Panel notes that there is a need for the Project analysts to articulate their position on waste package behavior and degradation modes. In support of this effort, the Panel recommends that white papers and critical reviews be prepared. These should include evaluations of relevant non-Project literature and experience from other applications.*

Response: The M&O is utilizing a detailed procedure for the development of analyses and models that describe each important waste package material degradation mode. These will include qualified data only; however, the data will be compared to relevant non-Project information as appropriate. Each important waste package material degradation mechanism will be described in a separate detailed technical document and all the information will be collected in the Waste Package Degradation PMR.

3.5 THE ROLE OF FUEL CLADDING

Comment 85 (pages 79–80): *Although general corrosion (oxidation) under dry, moist, or wet conditions at temperatures below 250°C will be extremely slow and failure by this mode is unlikely, other mechanisms of failure remain to be investigated experimentally: 1.) pitting and crevice corrosion; 2.) hydride-induced cracking; 3.) "unzipping" of cladding due to secondary phase formation (e.g., U_3O_8 or higher oxy-hydroxides of uranium). At present, there does not appear to be a set of studies available by which one can rule out the possibility of crevice corrosion in Zircaloy.*

Response: See the response to Comment 13.3.

Comment 86 (page 80): *Future experimental work may provide the necessary substantive basis for claiming credit for cladding; but these studies are not presently available. The lack of repository relevant data is further compounded by the fact that, as far as the Panel is aware, the U.S. program at Yucca Mountain is the only program which claims credit for cladding as a barrier to radionuclide release.*

Response: See the response to Comment 29.

Comment 87 (page 80): *The Panel notes that in addition to its continued concerns about the lack of relevant data that are required for the evaluation of the long-term behavior of Zircaloy cladding, other review bodies have expressed reservations and concerns similar to our own.*

Response: There is a wealth of information on the behavior of Zircaloy cladding and zirconium alloys under conditions that are relevant to the repository. However, the M&O agrees that there is uncertainty in the environment that the cladding will be exposed to in the long term. An effort

to understand the potential environments is underway that should provide the basis for understanding long-term behavior.

Comment 88 (page 81): *Issues that still require evaluation include:*

- *The condition of the Zircaloy cladding on arrival at the repository and prior to emplacement;*
- *More explicit definition of the geochemical environment during potential corrosion events, particularly within the waste package;*
- *An evaluation of hydride formation due to cladding interaction with steam or with hydrogen generated during the corrosion of the waste package or steel components in the fuel assembly; and*
- *More experimental investigations of cladding to determine whether additional failure mechanisms should be included in the analysis.*

The Panel notes that the project team has made full and effective use of the data available in the literature, but the lack of repository-relevant data remains a serious limitation to the credible, substantial use in the analysis of cladding as a barrier to radionuclide release.

Response: The condition of the cladding on arrival at the repository will be evaluated, using information in the literature. The M&O is also supporting an NRC/Electric Power Research Institute/Utility study that is focused on the examination of spent fuels in storage at the Idaho National Engineering and Environmental Laboratory from the dry storage demonstration program.

The M&O agrees that a more explicit definition of the geochemical environment during potential corrosion events is needed. The M&O has added analyses for in-package geochemical modeling. This work builds from the geochemical modeling performed in support of in-package criticality modeling. A modified version of EQ3/6 is being used to investigate the range of fluid compositions and phase assemblages that could result from degradation of the waste package and internal components. Varied input parameters include the fluid flux, assumptions for the partial pressures of O_2 and CO_2, and corrosion rates for fuel, glass, and metals. Some of the issues investigated have included the thermodynamic data for Cr-Fe corrosion products and the sensitivity of the system to the HLW glass composition. Separate calculations are being performed for the commercial spent fuel waste packages and the co-disposal packages for vitrified HLW and DOE-owned spent nuclear fuel.

The M&O is currently reviewing its position regarding the potentially active degradation mechanisms for cladding. It is believed that all relevant mechanisms have been considered. Some testing may be required to confirm Project assumptions.

Also, see the response to Comment 13.

Wilson (1985, 1987, 1990) performed three series of tests on the effect of cladding on fuel dissolution. One test used distilled water and the other two used J-13 groundwater. Additional

fuel tests with cladding are ongoing, as are the corrosion tests, and the delayed hydride tests and SCC tests are planned. A survey of corrosion tests in various salt environments is also being performed.

3.6 WASTE FORM DEGRADATION

Comment 89 (pages 84–85): *In its present form such a model is not transparent, traceable or testable. The primary difficulty is that the TSPA-VA analysis has not built an abstracted model on a process-based model that is founded on a broad set of experimental data (from both inside and outside the Project) and for which uncertainties can be analyzed on the basis of the data or the conceptual models used to describe the corrosion and alteration processes... . No broad and consistent picture of the behavior of spent fuel over time has been developed in the context of experimental studies of which there are many ... or in the context of natural analogue studies... . Certainly, numerous studies already exist in the literature that could have been used to make the case for and test the validity of the models used in the TSPA-VA, but this has not been done.*

This is an important short-coming of the TSPA-VA analysis because a major portion (>95 percent) of the radioactivity is contained in the UO_2 of the spent fuel... . The response surface approach provides little opportunity for testing and challenging the conceptual models which should form the basis of process-based models.

At present the following parameters are expected to affect spent fuel corrosion rates, the resulting formation of alteration products, and the related release of radionuclides into solution: Eh, effective surface area (geometric vs. grain boundary), pH, solution compositions, solubility-limiting phases, colloid formation and radiation effects on alteration phases and colloids. In the TSPA, these parameters have not been discussed in terms of a deterministic model which can then be used for a subsequent abstraction.... The detailed analysis and evaluation of models in the TSPA-LA should include a discussion of these controlling parameters. At the moment there are only limited data available for analysis; and in the absence of appropriate experimental programs, there can be no quantitative analysis or confirmation of the conceptual models.

Response: The M&O has spent a number of years collecting data on the dissolution of UO_2 in commercial spent nuclear fuel under conditions directly applicable to the potential Yucca Mountain repository. An empirical model based on a regression fit to this data was used by the M&O in the performance assessment modeling for TSPA-VA (DOE 1998a). The release rates of moderately soluble radioisotopes such as ^{237}Np are not controlled by the rapid alteration rate of the commercial spent nuclear fuel matrix. Only the release rates of highly soluble radioisotopes, such as ^{129}I or ^{99}Tc, are influenced by the alteration rate of the commercial spent nuclear fuel matrix. Even in this situation, the solubility of ^{99}Tc controlled its release in about half of the sample runs in TSPA-VA (DOE 1998a) rather than the alteration rate of the matrix. Therefore, although the M&O plans to reexamine the regression analysis when it documents the model for the TSPA-SR/LA, the M&O does not plan an extensive effort to build a process model of UO_2 from which to abstract results. Rather, the same approach as used in TSPA-VA (DOE 1998a) will be used for the first iteration of TSPA-LA. However, the M&O acknowledges that it is important to provide a general qualitative description of the mechanisms involved and how they are influenced by Eh, pH, etc., as the commercial spent nuclear fuel alters, and there are

plans to do so. Furthermore, the M&O will attempt to qualitatively relate the various mechanisms to various empirical terms to demonstrate the reasonableness of the model.

Information relevant to spent fuel behavior over long time periods will be taken from a number of natural analogue sites, including Cigar Lake, Oklo, Tono, Peña Blanca, and others, and will be incorporated into the Natural Analogue Synthesis Report in Fiscal Year 99. The site most analogous to Yucca Mountain is Peña Blanca, where conditions are arid, oxidizing, the uranium deposit is high grade, and it is young enough such that almost no Pb has entered the system. The other sites are not direct analogues to the overall Yucca Mountain system, but they provide an excellent database from which to model and understand alteration and dissolution of UO_2 and the formation of secondary phases.

Comment 90 (page 85): *For other waste forms, such as ceramic spent fuel, corrosion models are extracted from rather obscure sources ... or dated sources... . The TSPA-VA and supporting documents (Chapter 6) simply fail to avail themselves of the current, relevant literature on process-based models for waste form corrosion.*

Response: The alteration rates for DSNF used in the TSPA-VA (DOE 1998a) were obtained from information gathered by and used in a performance assessment conducted by Sandia National Laboratories in 1994 and 1997 (Rechard 1995, Vol. 2, pp. 11-12; 1998). This performance assessment work was funded by the NSNFP under the direction of the Office of Spent Fuel Management of the Assistant Secretary of Environmental Management of DOE. The alteration rates were based entirely on literature values. The NSNFP was aware at the time that these literature values would need to be substantiated by experiments and has been funding such work. The NSNFP plans to provide an appropriate model of alteration to the M&O, based on dissolution experiments of N-Reactor fuel in time for the first iteration of the TSPA-LA. The N-Reactor spent nuclear fuel represents 88 percent of the DSNF (in turn, all of the DSNF represents only about 3 percent of the 70,000 metric tons of heavy metal allowed for the potential repository). Hence, similar to the TSPA-VA (DOE 1998a), the alteration model for N-reactor fuel will be used to bound the alteration rates of all other DSNF in TSPA-LA.

Comment 91 (pages 85–86): *Additional analyses and "side calculations" are completed which use more advanced conceptual models and codes (e.g., the general reactive-transport code AREST-CT). Such codes account for a wide variety of relevant processes ... and do, to a limited extent, provide model results which are corroborated by experimental data, but there are major caveats (many noted by the project team, page 6-129) which limit their usefulness*:

- *Most of the required thermodynamic and kinetic parameters required for the models are not available.*
- *The identification of phases which result from spent fuel corrosion is still preliminary and incomplete.*
- *The identification of the phases which incorporate important radionuclides, e.g., ^{237}Np, is uncertain or tentative.*

- *The effects of the corrosion of the fuel assemblies on the interior of the canisters are not considered.*

- *The long term stability of the secondary phases has not been evaluated.*

- *The number of simulations is limited and important effects, such as variations in water composition, have not been fully evaluated.*

Finally, we note that the presentation of the spent nuclear fuel corrosion models and these side-calculations leaves much to be desired in clarity and transparency. It is difficult to clearly identify when models or codes are used only for side-calculations versus their inclusion in the TSPA-VA.

Response: The M&O will be sensitive to the need to improve the presentation and clearly identify any side-calculations in the documentation for TSPA-LA.

Comment 92 (page 86): *The Yucca Mountain Repository is mainly a repository for the disposal of the UO_2 in spent nuclear fuel. By volume and total activity, this is the most important part of the source term for radioactivity at Yucca Mountain. A carefully developed, thoughtfully presented, and critically tested model for spent fuel corrosion should be the basis for the TSPA-LA.*

Response: The M&O's objective is to provide a model for the behavior of spent fuel that is technically sound and based upon available Project and literature performance data. The model will include the appropriate degradation mechanisms for the cladding and the surface area of the spent fuel that is potentially exposed over time. The model will also include the alteration and dissolution of this exposed fuel and the transport of radionuclides from the fuel. It is unlikely that a major spent-fuel testing program will be performed. However, some short-term testing may be performed to confirm some conclusions. In addition, natural analogue data will be utilized where applicable.

Comment 93 (pages 86–87): *In order to address some of the issues raised above, we recommend specific efforts be directed toward:*

- *Better definition of the composition of the water that seeps into the waste package and a determination of how this chemistry is modified by reaction with the waste package.*

Response: The M&O agrees that this information is needed. An effort is underway to understand the environments that will occur over time within the waste package. However, sensitivity analyses indicate that in-package chemistry is relatively insensitive to the initial water composition, but is more sensitive to the water flux, the amount of evaporation, assumed gas fugacities, and corrosion rates.

- *An evaluation of effect of the corrosion products on the spent fuel.*

Response: The M&O agrees that this information is needed. An effort is underway to better understand the alteration of spent fuel as it is exposed to seeping water or water vapor. Work has started to evaluate the potential for unzipping due to high-temperature water vapor or to dripping

silicate-containing water. In addition, some information is available in the literature on water interactions in defective fuel rods.

- *The effect of alpha-radiolysis on the corroding fuel surface and on the corrosion products.*

Response: The current series of tests being conducted utilizes fuel recently removed from a reactor. Thus, both gamma and alpha radiolysis effects are part of the testing matrix, and tend to be conservative. In addition, a recent literature review has indicated that alpha radiolysis on spent fuel dissolution is a minor effect.

- *The formation of colloids on the corroding fuel surface.*

Response: The M&O agrees that this information is needed. The mechanistic basis for colloid formation, stability, and transport, in general, will be more thoroughly discussed as a framework for discussion of the Project results. Colloid characterization, quantitative colloid stability measurements, and dissolved and colloidal spent fuel radionuclide release measurements are continuing. Quantitative measurement of radionuclide attachment and detachment rates for a variety of natural and waste-form colloids is also continuing. This work, when added to the data in the literature and data being collected within other DOE projects, will form the technical basis for a revised colloid-associated radionuclide transport abstraction. It is anticipated, however, that collection of basic mechanistic parameters for colloid formation, radionuclide attachment, and colloid interactions with stationary materials, will continue into the confirmation period.

- *A better definition of the pathways by which water from the corroded spent fuel may escape from the engineered barrier system*

Response: Laboratory work is underway to establish an improved understanding of water flow in the engineered barrier system, including 1/4-scale drift hydrology tests with simulated waste package and drip shield barriers. Bench-scale tests are also underway to evaluate the hydraulic and transport properties of backfill and invert materials. Work is also underway to validate flow and transport models with test data and to analyze flow and transport paths in the engineered barrier system. This work will form the basis for model abstractions into the TSPA-SR/LA.

Comment 94 (page 89): *The most important parameter in the corrosion model is the value assumed for the* $k_{long\ term}$. *Parametric values can only confidently be obtained from long-term experiments (lasting years). Additionally, confidence in extrapolating behavior of corroding borosilicate glass would be greatly enhanced if a mechanism can be identified for this long-term process. Such knowledge could provide the basis for using bounding calculations for glass corrosion.*

Because of the enormous amount of previous work on glass dissolution and the data available in the literature, one should reasonably expect that the TSPA-LA will include rigorous comparison of these data sets to the models used in the TSPA-LA.

Response: Although the form of the equation for dissolution of the glass encapsulating HLW is not in contention, the M&O acknowledges that the data used for setting the model parameters in

the TSPA-VA (DOE 1998a) were limited in scope. The data came mostly from dissolution studies on glass compositions and HLW mixtures from the Savannah River Plant. To broaden the range of glass compositions for Fiscal Year 99, the M&O will evaluate the vapor hydration and aqueous dissolution of glass compositions and HLW mixtures from Hanford. This work on Hanford glass will be completed in time to be included in the first iteration of the TSPA-LA. Although this work will likely be followed by other tasks that will attempt to broaden still further the data used to set the model parameters, the first iteration of TSPA-LA will not include an extensive study of literature values. However, a simple comparison of the TSPA-LA data with literature values will be possible.

The M&O has been conducting long-term dissolution tests of borosilicate glass for over twelve years. Long-term rates have been measured and will continue to be measured. The M&O is also performing short-term tests to compare the dissolution rates to those that occur in the long term. In addition, the M&O has been utilizing conservative forward rates in its TSPA calculations.

3.7 RADIONUCLIDE MOBILIZATION

Comment 95 (pages 90–91): *The conceptual model used to define solubility-limited concentrations of radionuclides is well founded. The difficulty in applying the conceptual model and the sources of uncertainty, however, are large due to:*

1. *The lack of definition of the geochemical conditions as defined by the NFGE models.*

Response: The M&O agrees that the solubility-limited concentrations should be tied directly to expected chemical conditions within the system. However, without a set of possible compositional environments, it is difficult to appropriately define the potential solubility controlling phases for radionuclides. The NFGE in the TSPA-VA (DOE 1998a) is the first attempt to assess the changes that might occur in the solution composition and gas conditions the waste form may experience. Further work in this area to bound the possible conditions and define a number of surrogate environments would allow improved definition of the solubility controls.

2. *Most of the experimental data used to establish the ranges of the radionuclide compositions in solution are based on laboratory data in which solution compositions were determined, but the solid phases were not identified.*

Response: The M&O agrees that speciation and solubility studies depend strongly on the characterization of both solution and solid-state compounds. Interpretation of solubility data without an understanding of the compounds results in incorrect thermodynamic data and inaccurate geochemical predictions for the actinide solubility limits. Predictions of the actinide solubilities based on oxidation state analogies may not be successful, especially for the hydrolysis of actinides, since the thermodynamics for hydrolysis reactions depend on the ionic radii.

3. *The database for the relevant radionuclide-bearing phases is extremely limited.*

Response: The M&O agrees that there is a lack of thermodynamic data for actinides in general. Especially lacking is a fundamental understanding of the aqueous chemistry of the tetravalent

actinides because of the enhanced difficulties of Pu colloid formation. An understanding of the Pu(IV) chemistry is essential because Pu(IV) solids may control the natural solubility and, thus, further studies are needed.

4. *The expert elicitations and the functional forms used to describe radionuclide concentrations in solution have only a limited amount of data to substantiate changes as a function of simple geochemical parameters, such as Eh, pH and carbonate content.*

Response: The M&O agrees that additional data would improve the ability to couple the dissolved radionuclide concentrations more directly to functional dependencies on compositional parameters. This would provide improved bases for the process-level models used for abstracting models of radionuclide source terms into TSPA.

5. *The conceptual model may not be applicable to the actual processes of phase formation, dissolution and radionuclide release. Reactive-transport models, such as AREST-CT, may provide a more realistic description of radionuclide release; however, the database for the use of such models is even more limited than that for the solubility-limited models.*

Response: The M&O agrees that there is significant uncertainty associated with the processes of secondary phase formation, dissolution, and subsequent radionuclide release. For this reason, the M&O's emphasis will be placed on a solubility-limited model for radionuclide release. Some work may continue on the secondary phase issue, but the primary goal of this work will be to provide additional assurance that the solubility-limited model is not underestimating radionuclide release.

Comment 96 (page 91): *The Project should take advantage of the work in other national programs.*

Response: The M&O agrees that the development of process-level models and abstraction processes would benefit from an integration of relevant work performed within the international scientific community in the area of waste form evolution and radionuclide solubility limits.

Comment 97 (page 91): *As noted by the Panel in its third interim report ... the reassessment of the Np concentration range is a reasonable interpretation of the experimental data presently available; however, the present data do not allow one to identify the dominant process(es) that control the Np-concentration in solution (e.g., precipitation, coprecipitation or sorption).*

Response: The M&O agrees with this assessment that the existing experimental data be augmented such that a clearer understanding of the controls on dissolved Np concentrations can be synthesized and used to assess the performance of the potential site in a more realistic manner.

Comment 98 (page 91): *Additionally, the Np-bearing phases that control the solution compositions should be identified in the laboratory experiments, and a thoughtful case should be developed for the assumption that this phase will control Np-concentrations in the repository environment.*

Response: The control of Np solubility by pure Np solids can be considered as the conservative approach to geochemical modeling of the Np solubility limits. The data give the upper concentration limit for an aqueous system (Efurd et al. 1998). More realistic assumptions based on the low concentration of Np in spent fuel and the presence of a U-matrix have to consider the co-precipitation of Np in a U solid phase. These secondary phases may be the more important solubility-controlling phases. Drip tests showed that Np will not be incorporated into U(VI) silicates, but, in the short-term, formed metastable U(VI) hydroxide phases. Potential uptake mechanisms could involve the implementation of Np into the crystal structure (which would have a longer retention than surface sorption alone) or scavenger-precipitation with mainly sorption reactions. An understanding of the Np uptake and of the nature of these secondary phases is not available. Therefore, the M&O has had to rely on a very conservative solubility model for Np.

Comment 99 (page 93): *As noted in the Panel's third interim report (Whipple et al., 1998), there are, at present, only limited data on the structures and stabilities of the phases that form as alteration products of UO_2.*

Response: The M&O agrees that this information is limited, particularly in regard to aqueous transformations. However, the ongoing work is giving a better understanding of these processes. In addition, work has just been initiated to evaluate the potential for unzipping due either to high-temperature water vapor or to dripping silicate-containing water. An analysis of the products formed will provide further elucidation into these processes.

Comment 100 (page 93): *Although there has been considerable recent progress in the description of the structures of the relevant phases ... the fundamental data requirements for the models used in the analysis (e.g., AREST-CT) fall short of what is required for a definitive analysis.*

Response: The M&O agrees that there is a shortfall in the data required and activities are underway to obtain some of the critical information. However, a conservative or bounding analysis may be all that is needed to make a defensible case for LA.

Comment 101 (pages 93–94): *Proper evaluation of the secondary phases will require:*

1. *A determination of the phases that form over the range of relevant conditions... . This work should be compared to phase assemblages and relative abundances as described in relevant natural analogue sites.*

Response: Spent fuel and UO_2 dissolution experiments have been conducted for over eight years. Phases for both materials have been observed and compared to those that have formed in natural analogues. Oxides and silicates compare favorably with those observed.

Information on the formation of secondary phase assemblages, their abundance, stability, and potential for incorporating radionuclides will be obtained from studies of natural analogue sites, as one information source, and will be incorporated into the Natural Analogue Synthesis Report in Fiscal Year 99.

2. *A determination of the extent to which critical radionuclides (^{239}Pu, ^{237}Np, ^{99}Tc, ^{79}Se and ^{129}I) may be incorporated into the structures of these phases should be based on systematic experimental data.*

Response: A study is currently underway to evaluate the location of these key radionuclides, particularly Np, in secondary phases. In addition, an effort is planned to investigate secondary phase daughters in natural analogues that could shed further light on this issue.

3. *The incorporation of radionuclides into the uranyl phases does not mean that they will be retained as long as the phase is present.*

Response: The M&O recognizes that the long-term stability of the secondary phases formed by incorporation of these key radionuclides may be limited. However, the formation of the secondary phases indicates that they are more stable than spent fuel. In addition, see the response to Comment 95.2.

4. *An evaluation of the thermodynamic stability and/or solubilities of these phases is required.*

Response: The M&O is currently evaluating the thermodynamic and solubility data in the literature. However, it is doubtful that a complete set of data will be available. Thus, a bounding or conservative assumption may need to be made for LA.

5. *If the Project continues to use reactive-transport codes, such as AREST-CT, then considerable effort will be required to determine kinetic rate constants for dissolution and precipitation reactions.*

Response: The M&O agrees with the Panel that the kinetics of representative secondary uranyl minerals should be determined through experimental studies. The current rate constants for three major uranyl minerals (schoepite, uranophane, and soddyite) were derived from SKB (Svensk Karnbranslehantering AB [trans. "Swedish Nuclear Fuel and Waste Management Co."]) experiments (Casas et al. 1994; Bruno et al. 1995; Perez et al. 1997). However, the kinetic information for Na-boltwoodite, a secondary mineral expected to appear in the Yucca Mountain Repository, is missing. As an approximation, experiments on uranophane were used to estimate the dissolution rate of Na-boltwoodite in the AREST-CT model calculations because uranophane and Na-boltwoodite have very similar crystal structures. A first-order approximation of the rate constants for major representative uranyl minerals would generate reasonable results for performance assessment, and experiments to provide such approximations could be completed in a few months.

6. *All of the alteration and precipitation reactions that occur during the corrosion of spent nuclear fuel will occur in a high radiation field. The effects of ionizing radiation and alpha-decay event damage should be determined.... The panel recommends that, in addition to the analysis, radiation effects be studied experimentally.*

Response: See the response to Comment 93.

Comment 102 (page 94): *...the Panel notes that in the distillation of the literature, the Project has a tendency to selectively use that information which carries a positive message for the analysis.*

Response: The M&O agrees that it is important to provide a balanced representation of information summarized from the literature. In the future, the M&O will make efforts to give full and balanced views of the matter being presented.

Comment 103 (page 96): *At present there is no convincing way to estimate the type, amounts or stability of colloids. Further, these properties will vary along the transport path.*

Response: Understanding and estimating the type, amount, and stability of colloids that might be generated at Yucca Mountain under thermal and ambient geochemical conditions is very difficult. The first attempts under ambient conditions were captured in TSPA-VA (DOE 1998a) using available literature data. As more is learned about the NFE geochemistry and the materials in the EBS, there will be a better understanding of what types of colloids might be generated. Furthermore, the M&O agrees that, presently, there is no good way to estimate the amount or stability of these colloids with the existing data collected from Yucca Mountain or in the open literature. To help address this issue, the colloid modeling and data collection team is developing new UZ and SZ predictive models for colloids this fiscal year.

Comment 104 (page 96): *...we simply note that the K_d values will be sensitive to parameters, e.g., pH, that are presently not included in the model... . The effect of pH variations has also been confirmed in field-scale studies of actinide transport... . In the absence of a well defined geochemical environment the uncertainties will be large... . Both of these judgments will be highly speculative unless geochemical boundary conditions limit colloid formation or sorptive capacity. All of these estimates introduce considerable uncertainty into the analysis.*

Response: The M&O agrees that K_d values are sensitive to specific local geochemical parameters (ionic strength, pH, changes in boundary conditions, etc.), and that these parameters are not well known or adequately reflected in present transport models. The colloid model being generated this fiscal year will account for more of these parameters. Therefore, as more is learned about the NFE geochemical conditions, the better the prediction of the colloid type, stability, and mobility, as well as the sorptive capacity of colloids at Yucca Mountain, will be. The M&O also believes that the effect of the degree of saturation in the rocks and its associated effect on K_d's will become an issue during licensing, (e.g., the assumption that regularly-measured K_d's do not change at low water contents, and, especially, how these are used to calculate the retardation factors). There are data showing that retardation and K_d's can change as the water content becomes lower, and it can change both ways, either becoming higher or lower depending upon the material.

Comment 105 (page 96-97): *The Panel suggests that when modeling complex phenomena where few data are available and parameter ranges are wide, it is not useful to do a sensitivity analysis which focuses on the expected doses.*

Response: The M&O agrees with the sensitivity analyses comments on dose. This fiscal year, much more effort is being applied to sensitivity analyses of the physical and chemical parameters that affect colloid formation and stability.

Comment 106 (page 97): *The efforts to reduce uncertainty and substantiate the models will require:*

1. *A consideration of colloid-facilitated transport of ^{237}Np, as well as Pu.*

Response: Field-scale tests at Busted Butte and C-wells are looking at Np and Pu (based on analogue elements and microsphere) colloidal mobility. Limited additional column and batch lab experiments with these elements have already been or are being completed this fiscal year. In addition, Atomic Energy of Canada, Ltd., has removed a cubic-meter block from Busted Butte and is running UZ radionuclide transport experiments with it in Canada.

2. *A considerable experimental database to confirm the behavior of actinides in the batch-scale experiments over a range of conditions.*

Response: The M&O is producing and amassing thermodynamic data on the key radionuclides of interest to TSPA in order to generate solubility response surfaces. These response surfaces will then be used in a model such as EQ3/6 to produce the solubility ranges for the key radionuclides over a variety of geochemical conditions that may be encountered at Yucca Mountain.

3. *Because experiments with Pu and Np will be time consuming and the results cannot be confirmed by field-scale tests, the Panel recommends that the Project utilize the experimental and field data to confirm that their TSPA-VA model captures the range of behaviors exhibited by the most abundant actinide at the Yucca Mountain repository, uranium, e.g., at uranium ore deposits, mill tailings, natural analogue sites.*

Response: The M&O has initiated an effort to review anthropogenic and natural analogue data from around the world, including a study of radionuclide transport at Peña Blanca, Mexico, using U-series mobility, and a review of colloidal mobility at Idaho National Engineering and Environmental Laboratory and the NTS. This information will support evaluation of the issues related to radionuclide transport. The Natural Analogue Synthesis Report in Fiscal Year 99 will summarize information on the range of behavior of uranium in many types of settings, including ore deposits, disseminated uranium (e.g., Palmottu and some northern Nevada deposits), mill tailings, and other analogue sites.

4. *The TSPA models should demonstrate that modeled results are at least consistent with observations of colloid transport of plutonium at the Nevada Test Site... .*

Response: A SZ colloid model is being developed for the NTS to explain the Pu transport observations there. This model will also be used in the SZ flow and transport process model being developed for Yucca Mountain. In addition, this model is also being used as the template for the UZ colloid model being developed for Yucca Mountain this fiscal year.

Comment 107 (page 97): *Finally, given the large uncertainties that will almost certainly remain even after a considerable amount of experimental and field work, the Project may want to consider design changes (e.g., use of backfill) that would limit or prevent transport of radionuclides by colloids.*

Response: The LADS process resulted in an M&O-recommended design that includes a drip shield, an invert that uses granular ballast in a steel framework, and backfill. These features offer an opportunity to divert or filter natural colloids before they contact the waste, to filter waste-form colloids that leave the waste package, and to sorb radionuclides from the colloids.

The design of the backfill and invert ballast (and their performance assessment models) will consider the first two of these potential roles. Because the thickness of the invert is insignificant compared to the UZ and SZ transport paths, sorption of radionuclides from colloids in the invert will not be considered in the design or performance assessment. The Level 3 Change Control Board has directed the design organization to select the backfill and invert granular materials with consideration of the thermal, hydrologic, and water chemistry buffering properties of the materials. The two components may be of the same or of different material, and may be homogeneous or composed of multiple particle sizes and/or compositions. The desired properties are high thermal conductivity (to limit WP internal temperatures), minimal capillary wicking of water toward the waste package, and buffering of the water chemistry to limit acid pH levels.

The drip shield has the function of preventing advective water contact with the waste package. As long as the drip shield performs this function, diffusive transport through the invert from juvenile-failure waste packages will be the only release mode. The thickness of water films on the invert ballast material and the nature of the point contacts between the particles will influence colloid and dissolved radionuclide diffusion through the invert. The diffusion coefficient in the invert may be low enough that this mode can significantly delay releases to the accessible environment. However, since overall performance does not rely on slow invert transport, a bounding approach will be taken to develop the performance predictions of transport through the invert. In contrast, the drip shield is considered a principal barrier (delaying the onset of aqueous corrosion of the waste package until after the thermal pulse), and its performance will be estimated with less conservative models.

Comment 108 (page 98): *The Panel recommends that the Project staff initiate a detailed, on-going review of the EBS models... . The present EBS analysis uses only limited experimental data and, more importantly, there has been no effort to demonstrate that such an approach produces reasonable results. This situation can be significantly improved by designing experiments to confirm the modeled results of the EBS.*

Response: The M&O is reviewing EBS and in-drift geochemical process models and initiating experiments, such as the 1/4-scale drift flow tests and bench-scale tests, to improve the EBS experimental data and their validation. This work will be documented in the EBS PMR.

Comment 109 (pages 98–99): *The EBS analysis is an example of the combined and confounding use of conservative and bounding analyses. As an example, although the lower half*

of the waste package is considered to be in contact with the invert materials (concrete and steel), the properties of the invert material are considered to be those of intact concrete. However, the waste package can only come into contact with the invert materials by the degradation of the pedestal and invert materials. As noted by the project staff, this is a conservative assumption for diffusive transport and a non-conservative assumption for advective transport... . In other parts of the analysis, similar questions arise as to the conservative or non-conservative nature of the assumptions. Concerning the use of placeholder K_ds, the TSPA-VA analysts note, "Without further data it is difficult to assess if these ranges are conservative or non-conservative, although preliminary work ... suggest that they may be conservative." Thus, there is no basis on which a confident judgment can be made as to the degree of conservatism in the analyses.

Response: The concrete invert was a complex component of the EBS in the VA design (DOE 1998b) and introduced several uncertainties with respect to flow, transport, and its impact on the transport properties of the underlying geosphere. Primarily for this reason, the concrete invert is not being considered in the LADS process. Instead, the focus is presently on a steel invert with granular fill. Credit for radionuclide sorption will not be taken unless a sorptive material is used.

Comment 110A (page 99): *There are also many unsubstantiated assumptions in the analysis:*

1. *"The amount of water in the waste form cell is assumed to be equal to the pore space of the rind of alteration products that forms as the UO_2 is converted into secondary minerals."*

Response: Work is ongoing to improve the spent fuel alteration and release model. This work includes the development of a conceptual model of dissolution based on Project and literature data and a comparison of models against the flow-through, batch, and unsaturated drip tests.

2. *"The mass of colloids within the WP cells was calculated by multiplying the concentration of colloids by the volume of water within the cell." Although this is a reasonable and straightforward calculation, the concentration of colloids is based on the ionic strength of the water as estimated using the NFGE abstraction.*

Response: The approach described was implemented to simplify the calculations. Because the ionic strength of the solution in the waste package may be higher than in the drift, this simplification predicted lower releases than would have been estimated if in-package ionic strength was used. However, once the colloids exit in the package, they would be subjected to an ionic strength similar to the NFGE ionic strength as the package seepage mixes with the larger volume of drift seepage. Furthermore, the uncertainties associated with the colloid formation and transport probably swamp the effects of in-package versus drift seepage ionic strength. In an attempt to be conservative, very large colloid partition coefficients were implemented in the TSPA. Finally, experimental and modeling work that focuses on the formation, stability, and transport of colloids is continuing.

3. *"The volume of the water within each invert cell was determined by multiplying the porosity of the concrete invert (10 percent) by the physical volume of the cell." Again, the methodology is straightforward, but the assumption that the porosity remains at*

10 percent is based on the assumption that the invert has the properties of essentially intact concrete.

Response: See the response to Comment 109.

4. *"The flow value for the advective connection was set to the seepage through the drift and is not scaled to the area of the pits and patches on the WP." Although this may be a reasonable assumption, the underlying basis is not apparent.*

Response: The wording of this assumption was somewhat misleading. The advective connection between the waste package and the invert was scaled to the area of the pits and patches. The seepage that did not go through the waste package was allowed to go through the invert and mix with seepage from the package.

Comment 110B (page 99): *For the purpose of review, it is difficult to judge the cumulative effect of these assumptions on the results of the analysis.*

Response: Because of a lack of data, several simplifying assumptions were invoked for the EBS component of the TSPA. As a result, it is difficult to judge the cumulative effect of these assumptions. To improve this situation, an integrated testing and modeling effort has been initiated to obtain a better understanding of important flow and transport processes in the EBS. The intent of this work is to reduce uncertainties, obviate the need for assumptions that have little technical basis, and help put a more consistent treatment of the important sub-processes in the EBS.

Comment 111 (page 99): *Although units of mass are not transparent in their impact on the analysis (fractional release would have provided more immediately useful information), the Panel concluded that the more detailed analysis within the EBS (i.e., at the scale of the drift) is useful and we recommend that it be more widely applied.*

Response: Detailed analyses of releases at the drift scale are useful and will be conducted and documented in the EBS Process Models Report for the potential SR/LA. A related defense-in-depth review has recently been conducted and efforts to quantify the impact of EBS components on long-term performance are ongoing.

3.8 UNSATURATED ZONE TRANSPORT

Comment 112 (page 100): *...the deviation of flow around the perched water zones, as has been assumed in the model, may underestimate the existing retardation potential and cause streamlines to by-pass potentially sorbing formations. As pointed out in the review of UZ flow, this assumption is in need of further evaluation and confirmation. The Panel believes that a convincing resolution of these two flow issues, namely, estimation of a reliable value for the matrix-fracture reduction factor, and validation of the assumptions regarding by-passing of the water around potentially sorbing formations, will add considerable confidence to the validity of the TSPA-VA UZ transport projections.*

Response: The fracture/matrix reduction factors have been primarily used to bring the flow model predictions for water saturation and capillary pressure into agreement for the welded tuffs.

The welded tuffs have low matrix permeability, such that the range of percolation flux passing through these units exceeds the capacity of the matrix to transmit the entire flow. Therefore, fracture-dominant flow is guaranteed regardless of what fracture/matrix interaction factor is used. This leads to the conclusion that the fracture/matrix interaction factor for the welded tuffs will not have a large impact on radionuclide transport. For the nonwelded tuffs in the Calico Hills, the fracture/matrix interaction factors are generally very moderate, in the range of 0.5 to 1. Due to the very low matrix permeabilities found in the Calico Hills zeolitic units, the flow through these units is either very restricted (due to lateral diversion) or dominated by fracture flow. The flow through the higher permeability Calico Hills vitric unit is predicted to be matrix-dominated. Therefore, except for the Calico Hill vitric unit, the fracture/matrix interaction factors cannot substantially alter the fracture/matrix flow distribution between the potential repository and the water table. In the present treatment, flow through the Calico Hills vitric is matrix-dominated. With regard to the diversion of flow around perched bodies of water, alternate conceptual models (i.e., vertically dominant flow through the perched bodies of water versus lateral diversion around the perched water zones) are being considered for future TSPA calculations.

Comment 113 (pages 100–101): *The outcome of the analyses summarized in the TSPA-VA indicates that most of the sorption is associated with the TS layers, which are located directly beneath the proposed repository. Because of the proximity of the proposed repository horizon to these layers, however, the potential for the alteration of sorption and water chemistry properties from present-day conditions, as currently assumed in the model, can be significant. This introduces an additional uncertainty, beyond the existing problem with K_d values, in the estimated ability of the UZ to retard radionuclides. The project staff has made important strides in identifying many of the relevant factors related to these issues. The complexity of the problem, however, particularly due to the interaction of the UZ with the NFE/AZ, requires considerably more work in order to reduce uncertainties to an acceptable level.*

Response: The M&O recognizes the uncertainties in the NFE water chemistry compositions. It may be necessary to perform additional work to address uncertainties in this area. The water chemistry in the NFE and altered zone after the thermal pulse is still an unknown. In addition, the water chemistry will be slowly modified by percolation into the drift as time progresses, in addition to degradation of the NFE materials in the EBS.

Comment 114 (page 101): *The project staff has considerably improved the modeling of colloidal transport... . Matching with field data will be required, however, to assess the importance of processes such as colloid filtration and remobilization. Adsorption of colloidal particles on surfaces, will also be mediated by the ionic strength through double-layer interactions. At this point, although the potential significance of colloidal transport has been demonstrated, its expected effect remains unclear.*

Response: The M&O fully agrees, and work at Busted Butte and the C-wells field tests will go a long way in addressing this concern about filtration and remobilization. The M&O also agrees that the full effect of colloid transport on TSPA performance remains unclear at this time. Radionuclide percolation box-transport experiments and the intermediate scale (cubic-meter block) UZ transport tests at Atomic Energy of Canada, Ltd., underway this year, will help understand this behavior better for TSPA-SR/LA.

Comment 115 (page 101): *A key simplification in the TSPA-VA abstraction is the specification of the source term for radionuclides released from the proposed repository. In the current model, release rates are averaged spatially and uniformly over six large areas, each corresponding to a different percolation flux, as specified by the infiltration maps. Under this assumption, the model equates the effect of several, isolated and non-overlapping plumes of small cross-section and high concentrations to that of a single plume of large area and inversely smaller concentration (so that the overall release rate remains constant). As noted below, the same problem arises in the treatment of SZ transport. The effect is equivalent to a lateral spreading, which artificially increases the dilution capacity of the UZ system, particularly during juvenile failures. The Panel believes that a more careful analysis of this problem is necessary to accurately reflect radionuclide spreading, particularly at the earlier stages of repository performance.*

Response: For the UZ transport model, the assignment of radionuclide releases to specific grid nodes at the repository is being developed. This will provide a better resolution of the radionuclide mass releases than the method used in TSPA-VA (DOE 1998a), where the mass releases were assumed to be spread uniformly over relatively large repository regions. This will result in a more accurate representation of radionuclide concentrations in the UZ transport model.

Comment 116 (page 101): *Other issues related to modeling, and which need to be resolved, include the effect of grid-scale* [heterogeneity] *on flow and sorption properties and its proper upscaling in a matrix-fracture dual continuum; the nature of the interaction under episodic flow conditions (namely whether flow is in the form of films, lenses, etc.); and the ability of the particle-tracking method to describe non-linear interactions, in which case, the RTD cannot be computed analytically.*

Response: Sub-grid scale heterogeneities may certainly impact the local behavior of flow and transport between fracture and matrix. While it is not possible to capture all aspects of localized heterogeneities, the attempt is being made to capture several processes, including fingering, fracture channeling, and even fracture coating—all of which act to reduce the amount of fracture/matrix interaction. The reduced fracture/matrix conductance to flow and transport can be accounted for in the particle-tracking method through the fracture aperture parameter. Other transport properties (e.g., diffusion coefficient, K_d) are treated stochastically to account for some of the uncertainty associated with upscaling.

Comment 117 (page 101): *Finally, the merits of the two different approaches taken for modeling transport in the UZ and the SZ, namely the use of particle-tracking vs. the use of an overall dilution factor, need to be compared. It is the Panel's position that a uniform approach should be adopted for both cases.*

Response: It is currently planned to use a streamline particle-tracking method for simulating radionuclide transport within the site-scale SZ coupled flow and transport model. In this way, transport in both the UZ and the SZ will be treated similarly in future TSPA evaluations and, in particular, the use of an overall dilution factor for the SZ transport simulations will be obviated.

Comment 118 (page 101): *...confidence in these numerical models to simulate real processes would be considerably enhanced if they could be confirmed by laboratory and field data.*

Response: The M&O concurs that confidence in the models would be enhanced through laboratory and field testing. See the response to Comment 2.

3.9 SATURATED ZONE FLOW AND TRANSPORT

Comment 119 (pages 101–102): *The current treatment of saturated zone (SZ) flow and transport at Yucca Mountain is far from satisfactory... . There are three main areas where important weaknesses can be identified in the current treatment:*

- *The lack of data for some important parameters*
- *The incomplete nature of site characterization*
- *Continuing questions regarding the adequacy of the numerical models.*

Response: The incomplete nature of the data from the SZ is being addressed through the wells that Nye County is drilling as part of its EWDP in the area where the Project has an identified data gap. In addition to providing geological and lithologic information, the wells will be used to monitor water level and sample water hydrochemistry, and to provide flow and transport parameter data through hydraulic and tracer testing. The data may be obtained from the following:

- Lithologic/geological logs from the new wells installed by Nye County in the identified data gap area
- Results from hydraulic testing of the hydrogeologic units penetrated by the new wells
- Results from hydraulic and tracer testing at a proposed alluvial testing complex
- Results from testing at the C-Wells Complex and laboratory measurements for matrix diffusion, dispersion, and sorption
- Results from laboratory and field testing of colloid-facilitated transport, including NTS data

It should be pointed out that a full 3-D, site-scale coupled flow and transport model is being developed to support TSPA evaluations for the potential SR/LA. The model domain is rectangular and extends from about 15 km north of the potential repository to about 30 km south of the potential repository and from about 15 km west of the potential repository to about 15 km east of the potential repository. Vertically, the domain extends from the top of the water table to a depth of 2,750 m and includes the upper part of the carbonate-rock aquifer system. This model is intended to replace the streamtube approach that was used in TSPA-VA (DOE 1998a).

Since TSPA-VA (DOE 1998a), the SZ numerical model has been improved to provide subsequent TSPA evaluations with a technically defensible model of groundwater flow and radionuclide transport from beneath the repository to the accessible environment. The source term at the water table may be large or small in extent. The source size will be conservatively

assigned to a small region (approximately 100 m x 100 m) that will not tend to overestimate dilution, as was inherent in the TSPA-VA (DOE 1998a) approach. The improvements to the model include:

- Enhancement of the hydrogeological framework through:

  - Incorporation of an updated geologic map and cross sections
  - Incorporation of geologic and hydraulic data from the Nye County EWDP wells

- Refinement of the model grid.

- Refinement of input parameters that includes improved lateral boundary conditions, allowance for non-uniform recharge over the model domain, and specified recharge along Fortymile Wash.

- Adoption of a transport modeling approach that uses a streamline particle-tracking methodology in the 3-D flow and a transport model which will not entail the implicit homogenization of the streamtube approach. The use of this 3-D transport methodology will provide the following capabilities:

  - Transport model calculations based on a full 3-D process-level flow model

  - Allowance for a wide range of dispersivity values, including very low values

  - Allowance for different source areas

  - Allowance for plume sizes of smaller dimensions than the grid spacing

  - Allowance for matrix diffusion and sorption transport processes

- Use of geostatistics to represent heterogeneities within the block cells and to investigate fast flow and transport pathways.

Comment 120 (page 102): *The lack of field data presents a major difficulty. There is a broad area along the projected SZ flow path from Fortymile Wash to the* [Amargosa] *Valley, 10 km or more in length, in which no boreholes have been drilled. For this region, there is a resulting absence of data on key subjects such as: subsurface geology, water table configuration, hydraulic parameters, etc.*

Response: See the response to Comments 2 and 118. Additional characterization of recharge has been completed. The 3-D SZ site-scale flow and transport model explicitly includes areal recharge over the model domain and the estimated recharge along Fortymile Wash.

Comment 121 (page 102): *In addition, one notes an apparent difficulty in estimating vertical flow in the SZ, the location of the lower boundary, and the lack of account for anisotropy and heterogeneity.*

Response: The apparent difficulty in estimating vertical flow in the SZ is now being addressed through the use of a 3-D flow model. The vertical flow in the SZ model is currently estimated through the use of conductance between as many as 16 model layers. Each model layer has a specified potentiometric surface and hydraulic conductance within each grid cell and between the layer and adjacent layers. This allows simulation of the vertical flow between model layers and, thus, an estimation of vertical flow in the SZ system.

Since TSPA-VA (DOE 1998a), the lower boundary of the SZ model has been deepened to coincide with a natural no-flow boundary and to maintain consistency between the regional and site-scale models.

Anisotropy is defined as the difference in hydraulic properties between the vertical and horizontal axes (vertical anisotropy) and within the horizontal axis (horizontal anisotropy). Anisotropy in the vertical direction is handled in the model through the anisotropy ratio between the horizontal and vertical hydraulic conductivities. The horizontal anisotropy is caused by the presence of flow-enhancing features and flow barriers (i.e., faults and fractures). The horizontal anisotropy is handled in the model through the direct representation of faults and fractures. Heterogeneity is handled in the model explicitly through the use of different hydraulic property zones in the numerical model, and implicitly through the use of geostatistics at the block-cell-scale and between block cells.

Since TSPA-VA (DOE 1998a), the model grid resolution has been improved by reducing the numerical grid size from that used in TSPA-VA (DOE 1998a) and by using a transport methodology, described above, that is not impacted by the grid size.

Comment 122 (pages 102–103): *...groundwater flow over the 20-km path from the repository site occurs mostly in the volcanic units and alluvium, and flow occurs in only 10 percent to 20 percent of the fractures. As indicated above, field data are needed to verify this picture of the SZ zone. Because K_d values in the matrix (especially for Np) can be 10 to 100 times higher than K_d values in the fractures..., it is necessary to know what percentage of the radionuclides are in the matrix of the volcanics. The division of flow in the fractured volcanics is one more aspect of the fracture-matrix interaction problem, the UZ aspects of which have been discussed above in sections IV A, B, and H. Finally, Gelhar (1998) has also indicated that K_d values cannot be used without knowing how representative they are of field conditions. Thus, we see that there is a serious lack of field data upon which to base the analysis of retardation.*

Response: The M&O agrees that more field data on fracture/matrix interaction are needed. The best data available for the potential SR and LA will be that from the niche seepage, Busted Butte, and the C-wells tests. Both the Busted Butte and C-wells data indicate considerably more fracture/matrix interaction than had been previously envisioned in either the UZ (up to two orders of magnitude) or the SZ. The M&O also hopes to have some data from the SZ alluvial complex by TSPA-LA, although most of the information from that test will arrive during LA review.

Comment 123 (page 103): *In the TSPA-VA, SZ site characterization affects primarily the description of the flow streamtubes, through the estimation of the permeability field and the water fluxes (in both SZ and UZ). The current approach for estimating the permeability field is*

based on the calibration of pressure heads. In addition to the problem of lack of data over a substantial region of the SZ as pointed out above, it is known... that pressure data inversion does not guarantee uniqueness in parameter estimates. Thus, potential fast paths in the SZ (such as permeability channels) may be underestimated. Obviously, the implications of such a possibility on the transport of radionuclides are significant and cannot be dismissed.

Response: Other than circumstantial evidence implicating Fortymile Wash as a structurally controlled preferential pathway within the SZ along the east and to the south of the site, there is little evidence for potential fast paths in the SZ down-gradient from Yucca Mountain. Solitario Canyon fault is a major block-bounding fault that apparently impedes ground-water flow from west to east across the fault and for which there may be some thermal evidence for upwelling groundwater along the fault. Additionally, the apparently low hydraulic gradient from north to south on the west side of the fault, specifically from boreholes USW H-6 to USW WT-10, may be evidence of a zone of relatively high lateral permeability in the hanging wall along the strike of the fault, which could be indicative of a fault-related north to south preferential pathway. Currently, there is no evidence that the other block-bounding faults, such as the Bow Ridge and Paintbrush Canyon faults, which may appear to be candidates for preferential flow pathways, exert significant influence on the SZ flow system in the site area. However, the existence of preferential flow pathways down-gradient from the site cannot be dismissed, and it is currently planned to allow for such features in the site-scale SZ flow and transport model through geostatistically based approximations. These approximations will permit bounds to be placed on the expected consequences for radionuclide transport to the accessible environment due to the presence of such features.

Comment 124 (page 103): *In the same context, there also exists the issue of numerical resolution in the modeling of regional flow, where only 3 vertical layers (spanning 2,750 m) are used to represent the large-scale hydrology and a typical grid has a linear (horizontal) size of the order of 1500 m. With such limited resolution, intra-grid heterogeneity is seriously misrepresented. The same remark also applies even for the site-scale model, which involves a grid resolution of 200 m. Given the large range in permeabilities, which spans 7 orders of magnitude, this limited resolution raises the issue of the relevance of numerical predictions regarding the postulated flow fields.*

Response: The shortcomings, including both lateral and vertical grid resolution, of the current regional SZ flow model are well recognized. These shortcomings are part of the reason for a decision by the DOE to join in an effort by Yucca Mountain Site Characterization Project and NTS to revise and refine the regional model. Unfortunately, results from this model are not expected to be available in time to support TSPA-SR/LA. The site-scale and regional modelers are working closely together, however, to expedite incorporation of the data and insights gained during development of the regional model into the site-scale SZ model.

The current site-scale SZ flow and transport model is based on a hydrogeologic framework grid resolution of 125 m and, for the flow and transport numerical simulations, on three rectangular computational grids with spacings of 1,000, 500, and 250 m. Results to date indicate that there is little difference in flow solutions between the 500-m and 250-m grids; however, the smaller grid spacing will be used for the radionuclide transport simulations. As in all large-scale modeling efforts, a balance must be sought between grid resolution, data availability, and computational

efficiency without, however, sacrificing adequate representation of the features and processes controlling the flow system. The expectation is that the grid for the site-scale model can be refined, especially in the area down-gradient from the site in which radionuclide transport would probably occur, as additional data, for example, from the Nye County EWDP, become available.

Comment 125 (page 103): *Given the uncertainties pertaining to the characterization of the site, the postulated flux multipliers for the future climates (4 for the Long Term Average and 6 for the Super Pluvial) are also uncertain. Streamtubes are assumed not to vary with time, regardless of the changes in climate, which is assumed to affect only the volume flux through them. This assumption is not consistent with the change in the ratio of the water flux through the UZ and the SZ zones....*

Response: The M&O recognizes that the problem discussed in this comment may be relevant. The simplifying assumption used in TSPA-VA (DOE 1998a) was that the flow paths in the SZ would not be significantly altered by climate change. This is contrary to data suggesting that the water table could be significantly higher under wetter climatic conditions and also inconsistent with the rise in the water table for the UZ transport analyses in TSPA-VA (DOE 1998a).

We plan to assess the significance of this simplifying assumption in a sensitivity analysis with the 3-D SZ flow and transport model for future TSPA modeling. A more complex representation of the impacts of climate change on SZ flow will be developed if the simplifying assumption is not supported by the sensitivity analysis.

Comment 126 (page 103): *In the current analysis, it is assumed that recharge along Fortymile Wash enters the groundwater to the east of the plume, but it does not enter on top of the contaminated water. Recharge on top of the projected flow path would alter the streamlines significantly, resulting in a substantial layer of clean water above the contaminated water. In his report to the* [N]*WTRB, Gelhar (1998) suggests that such a layer could be 100 to 150 meters thick. This potentially conservative feature would call into doubt the basic biosphere model, in which a farm family is assumed to pump contaminated water from the plume.*

Response: The 3-D SZ site-scale flow and transport model explicitly includes an estimated recharge along Fortymile Wash, so the effects of this feature will be included in the TSPA analyses. However, the NRC draft 10 CFR 63 (64 FR 8640) regulations do not include any assessment of the probability that the contaminant plume will be intercepted by wells in the receptor population. The increase in the depth of contaminated groundwater by 100 to 150 m clearly does not render the groundwater inaccessible. The M&O considers that it would be very difficult to argue that it is possible to ignore the risk associated with this deeper contaminated groundwater.

The current conceptual model regards Fortymile Wash to be a preferential pathway of local high transmissivity in the SZ to the east of the potential repository that channels water southward relatively rapidly. Under this conceptual model, water in the SZ moving eastward from beneath the potential repository would be deflected southward as it approached the Fortymile Wash pathway. Water recharging in Fortymile Wash would not enter the SZ on top of any contaminant plume emanating from beneath the potential repository. In this model, one should envision water in the subsurface Fortymile Wash pathway as sliding rapidly past the slower

moving ground water to the west of the pathway with the boundary between the two zones of rapid and slow ground-water flow being analogous to a transform fault.

Comment 127 (page 104): *Since the Project staff has similarly provided overall dilution factors instead of a more detailed analysis, the net result is that the interaction of plumes containing different radionuclide concentrations is also treated inadequately, in a generally ad hoc manner. The Panel believes that a numerical approach based on a streamtube formalism, well-resolved near the plume and with a correct representation of dispersion and retardation, is feasible (provided that a good description of the heterogeneity from field data is available).*

Response: The manner in which the interaction of radionuclide concentrations among the streamtubes in TSPA-VA (DOE 1998a) is not physically realistic is acknowledged as such in the documentation. However, it is shown that the method used is the only feasible method that is not non-conservative within the context of the multiple streamtube approach. In addition, a sensitivity analysis is provided that assesses the approximate degree of conservatism associated with the method accounting for interaction among the streamtubes (i.e., summing concentrations).

The streamline particle-tracking method that will be used in future TSPA modeling retains the advantages of the streamtube method, while allowing greater flexibility and physical realism. Streamline particle tracking is essentially the tracing of a streamtube in the groundwater flow field. Random walks of the particles simulate the effects of dispersion.

Comment 128 (page 104): *At the same time, this matter also brings up the question ... of why the modeling of the transport problem is treated differently in the UZ (using a particle-tracking method) and in the SZ (using streamtubes with a dilution factor). A unified treatment should be feasible and should be adopted.*

Response: The site-scale SZ flow and transport model currently under development to support TSPA-SR/LA will use a streamline particle-tracking methodology to simulate radionuclide transport. It is similar to what is used by TSPA-VA (DOE 1998a) to simulate radionuclide transport in the UZ. This methodology will allow for hydrodynamic dispersion, sorption, and matrix-diffusion processes to be included in the SZ transport calculations.

Comment 129 (page 104): *In the TSPA-VA model, flow is assumed to occur only through the fractures, the water in the matrix being stagnant. Instead of explicitly modeling mass diffusion from the fracture to the matrix, the approach taken is to introduce an effective, time-independent porosity for the entire system, in which low porosity values reflect small diffusion, and high values reflect a more enhanced diffusion. The problem with this representation is that the degree of fracture-matrix interaction is fixed a priori, rather than being a time-dependent process as it is in reality. Given that retardation is associated with the matrix, this assumption will affect the transport predictions.*

Response: The streamline particle tracking method that will be used in the 3-D SZ flow and transport model is being coupled to an analytical solution for matrix diffusion into finite-domain matrix blocks. Future TSPA analyses will explicitly simulate diffusion from fractures into the matrix, based on specified values of fracture spacing.

Comment 130 (pages 104–105): *We finally note the issue, also raised in the discussion of UZ transport, of averaging the source concentrations over six areas, which here lie at the interface between the UZ and the SZ. As in UZ transport, this assumption introduces an artificial spreading which will lead to non-conservative estimates, particularly at early times (e.g., within the first 10,000 years) when leakage of radionuclides from waste packages is associated with isolated failures. For such failures, the Panel suggested in its third interim report that it is unrealistic to assume that radionuclides will produce a uniform concentration in the groundwater beneath the repository across a flow path that is hundreds to thousands of meters wide.*

In response to the Panel's criticism, the M&O conducted a sensitivity analysis (Arnold and Kuzio, 1998) of the effect of the source size on the dilution factor at the 20-km point. In this analysis, the degree of non-conservatism introduced by the approximation made in the TSPA-VA can be assessed. It was found that, as a result of this approximation, the TSPA-VA underestimates the dose rates, for the base case parameter values, by a factor of 3. A correction was not introduced in the TSPA-VA, however. The Panel agrees with the general results of Arnold's analysis, and recommends that the current TSPA-VA treatment be modified to correct the existing deficiency. In particular, the method described in the sensitivity analysis by Arnold and Kuzio (1998) should be applied to the assessment of exposures that would result from human intrusion and from the juvenile failure of a waste package.

Response: See the response to Comment 7.

3.10 BIOSPHERE

Comment 131 (pages 105–106): *Although the treatment of the biosphere analyses in the TSPA-VA represents an improvement over previous such efforts, much work remains. From the perspective of the Panel, the sequence of steps in the biosphere segment of the performance assessment should have included an:*

- *Initial identification of the key radionuclides and pathways through which they could cause exposures of neighboring population groups*
- *Identification of the key parameters affecting the associated dose estimates*
- *Initiation of a concentrated effort to confirm site-specific values for each of these parameters as well as their associated uncertainties*
- *Confirmation of the preliminary identifications and associated dose estimates.*
- *Although the first and second steps in this process were completed, it is the conclusion of the panel that far too little effort was directed to the third and fourth steps. Specific needs include*
- *Increased efforts to ensure that advantage has been taken of all biosphere relevant information that is available in the published literature.*

- *Conduct a systematic supporting effort to measure in the field or, if necessary, in the laboratory, site-specific values for the key parameters needed as input to the biosphere environmental transport and dose assessment models. Where such studies are impractical or cannot be performed, efforts should be made to estimate appropriate values based on knowledge of the characteristics of the environment in the vicinity of Yucca Mountain.*

- *Assessment of the uncertainties and conservatisms associated with the values for each of these parameters.*

Integral to the success of these efforts should be a willingness to challenge "conventional wisdom" such as the assumption that ^{129}I deposited in the soil through the use of irrigation water will not be absorbed ... there was relatively little effort to obtain site-specific data on the key radionuclides that determine the dose... . Where field data were not available, or could not readily be obtained, estimates should have been made using knowledge of the properties of the site and region....it is not always obvious whether a site-specific or default value was assigned to a given input parameter. Even in those cases where it is known that a default value was used, it is not easy to ascertain the assigned numerical value.

Response: Biosphere analyses conducted in support of TSPA-VA (DOE 1998a) used data that were site-specific where such data were available. In lieu of site-specific data, TSPA-VA (DOE 1998a) used data that were considered relevant and representative of the environment around Yucca Mountain. The M&O is committed to the use of site-specific and relevant data that were not considered in TSPA-VA (DOE 1998a). Analyses planned to support TSPA-SR/LA will identify key radionuclides and pathways that contribute to the projected dose. Attempts will be made to include uncertainty analysis and to address the subject of conservatisms associated with the values of the parameters used in bioshpere modeling. See, also, the response to Comment 133.

Comment 132 (pages 106–107): *...the Panel believes that more attention should have been directed by the TSPA staff to the GI absorption factor for each key radionuclide... . the Panel recommends that the TSPA staff critically review the values that were used in setting the dose conversion factors in the FGRs No. 11 and No. 12. Of particular interest is how these factors vary depending on the chemical nature of the radionuclides.*

Response: Biosphere assessment activities were conducted in accordance with accepted methods for the demonstration of regulatory compliance. The GI model used in this assessment is consistent with that used in Federal Guidance Report No. 11 (EPA 1988). Examination and critique of this model was outside the scope of the TSPA-VA (DOE 1998a) effort. For SR/LA, the M&O will complete the biosphere analyses in accordance with relevant regulatory guidance.

Comment 133 (page 107): *...it appears that, for several of the radionuclides, the assigned values for the previously discussed gastrointestinal absorption factors are extremely conservative. Even in those cases where the conservatisms were identified, the TSPA-VA staff made no attempt to quantify them. In a similar manner, the staff acknowledged that the dose conversion factors used in making dose estimates contain uncertainties. Again, however, they did not attempt to quantify them... . If the analyses were restricted to the key radionuclides and*

the key exposure pathways, the required effort might readily be manageable... . It would appear that the quantification of the conservatisms and uncertainties would be an important step as the TSPA staff approaches the LA stage... . Having such information would appear to be essential in determining whether the results of the analyses provided "reasonable assurance" that the regulatory requirements have been met.

Response: The assessment in TSPA-VA (DOE 1998a) did not address the conservatisms and uncertainties associated with values established through consensus and accepted by the scientific community (e.g., dose conversion factors and associated parameter values) because they are independent of the biosphere considered and, hence, were beyond the scope of that effort. TSPA-VA (DOE 1998a) did consider the uncertainties associated with many of the parameter values, both site-specific and published, that were used in the calculations. Quantification of the impact of conservatism and uncertainty on dose projections would improve future assessments. As a result, planning activities are currently underway to determine the extent to which conservatisms and uncertainties could be quantified in TSPA-LA.

Comment 134 (pages 107–108): *No retardation credit is taken for ^{99}Tc and ^{129}I (or for three other radionuclides), based on the lack of observed sorption in batch measurements of K_d values in the laboratory. This decision is described in the TSPA-VA as being conservative. However, field measurements near the Savannah River Plant and in the vicinity of the Chernobyl nuclear power plant, following the accident at that facility, indicate that radioactive iodine deposited on the ground has been retained in the upper soil layer to about the same extent as were plutonium and cesium... . The panel has not conducted a literature review on this issue, but it seems likely that measurements taken of areas near the Chernobyl site, for example, would also provide relevant data on the retention or lack of retention of technetium in soil... . It is the Panel's view that the Project staff, in preparing the TSPA-VA, unduly emphasized the results of laboratory K_d measurements, and did not appropriately consider the results of field measurements of radionuclide concentrations in the soil following releases that occurred as a result of nuclear power plant accidents and past nuclear facility operations.*

Response: The M&O agrees with the Panel's concern and plans to examine field data on the retention and buildup of radionuclides in soil and other substrata from other sites. See, also, the response to Comment 20.

3.11 EARTHQUAKES, VOLCANISM, CRITICALITY, HUMAN INTRUSION, AND CLIMATE CHANGE

Comment 135 (page 108): *For purposes of the analysis of the impacts of seismic events on repository performance, the TSPA-VA staff has concentrated on scenarios in which postulated rockfalls may damage a waste canister. For other seismic effects, including flowfield disruption, effects of fault displacement, and groundwater-level rise, the staff has asserted with plausibility arguments, rather than with detailed analysis per se, that the impacts would be minor. The supporting analysis in these areas, however, are as the staff admits, only of a scoping or screening nature. The arguments that are advanced may be reasonable, but the analysis lacks a documented, convincing rationale. Such a rationale will be necessary for the LA stage, if the Project progresses this far.*

Response: Features, events, and scenarios for seismic activity will be reviewed and screened as part of the analysis process for SR/LA. These include the features, events, and processes for performance assessment of the consequences of flow-field alteration, fault displacement, and water table rise. The M&O agrees that it is important to provide a documented rationale for excluding these specific seismic effects. For SR/LA, the M&O will conduct and document technical analyses to support the screening (i.e., inclusion or exclusion) of specific features, events, and processes. The screening methodology is summarized in (DOE 1999).

Comment 136 (page 108): *Further complicating the analysis is that efforts have been made to examine effects for a full 1,000,000-year time horizon. This has apparently consumed so many resources that a thorough exploration of the first 10,000-year period has not been done adequately. As a result, the more robust insights about the 10,000-year time horizon that might have been developed are not available.*

Response: The process model for rockfall will be refined for SR/LA. This will include integration into WAPDEG and treatment of juvenile failures. There is still little evidence that rockfall can cause failures in the first 10,000 years because of the relatively small sizes of rock expected to fall in the drifts, the robustness of the waste package materials and construction, and the proposed addition of a drip shield.

Comment 137 (page 110): *Defending the acceptability of the proposed repository during the regulatory review phase will undoubtedly require that much more attention be directed to evaluating rockfall effects during the first 10,000-year period.*

Response: The M&O agrees that the analysis of rockfall events during the first 10,000 years after the repository is closed needs to be strengthened. This is planned for future performance assessment analyses for rockfall.

Comment 138 (page 112): *The effects of volcanism on overall repository performance seem to be acceptably small in terms of their relative contribution, but the technical disagreements with the USNRC analysis need to be resolved.*

Response: The M&O agrees that the technical disagreements with the NRC on the probability and consequence of volcanic activity need to be addressed. The DOE and the NRC have an ongoing effort to resolve issues related to volcanism. This year, they held Appendix 7 meetings and workshops in early 1999 to work on resolving the technical disagreements.

Comment 139 (page 114): *One inconsistency with other aspects of the TSPA-VA analysis is the treatment of so-called "juvenile" canister failures, which seem to be ignored in the criticality analysis.... It seems obvious to the Panel that there is at least some small probability that such a juvenile failure could produce the bathtub configuration that is the starting point for the in-canister criticality analysis. Such a possibility, however, was not evaluated in the TSPA-VA. In the opinion of the Panel, this should have been done.*

Response: As part of the enhanced/revised/improved waste-package analyses, juvenile failures will be considered in more detail. As noted in the response to Comment 61, additional analysis of the data and models on juvenile failures is ongoing. The essence of future criticality analyses

by the M&O will be to review the probabilities that could lead to conditions favorable for criticality. These will, of course, include juvenile failures.

Comment 140 (page 115): *To be specific, more work will be needed to support the conclusion that the occurrences of criticality outside the canister are of no importance, and to demonstrate that the in-canister scenario selected is bounding. In addition, the in-canister scenario needs to be refined.*

Response: The screening activity for features, events, and processes for the potential SR and LA will evaluate the potential dismissal of the external criticalities using both probability and consequence arguments. Similarly, the intent is to use probability arguments to screen out in-package criticalities during the first 10,000 years. The results of these screening activities will be thoroughly documented for SR/LA.

Comment 141 (page 116): *The scenario selected by the TSPA staff is admittedly unrealistic. This is especially true in terms of certain of the associated extremely conservative assumptions. Examples include the fact that, using today's drilling technology and practice, most of what any drill bit strikes would be brought up to the surface, not sent down to the bottom of the hole. It is also assumed that the volume of material sent down to the SZ includes not only that which is directly removed by the drill, but also a considerable amount of the surrounding material. In fact, the estimated mass that is transferred is between about a half-ton and nearly three tons. Although these assumptions do not represent an unreasonable starting point to scope-out the issues, in the Panel's judgment they appear to be too conservative. As a result, estimates of the resulting impacts (doses) are much higher than would actually be the case.*

Response: The M&O agrees with the Panel's comment. The scenario selected for TSPA-VA (DOE 1998a) was, however, consistent with the NRC proposed rule 10 CFR Part 63 (64 FR 8640). Future human-intrusion scenarios will include an analysis of the effects of an improperly sealed borehole as a fast path for water flow through the repository to the water table. Analyzing the performance assessment effects of an open borehole will permit considerations of repository-specific processes that can be used to test the resiliency of the potential repository to human intrusion.

Comment 142 (page 116): *Based on the capabilities of today's drilling technology, the analysis of how much material is intercepted or disturbed by the drill bit seems reasonable. That is to say, the Panel believes that the TSPA staff has carefully considered how to handle the spallings issue and the associated issue as to how much additional material beyond the diameter of the hole cut by the drill bit, itself, will be disturbed. Overall, the analysis appears to be conservative but reasonable. In contrast, the SZ analysis is, in our view, incorrect. This is due to the fact that, as discussed elsewhere in this report, the model used in the SZ analysis is inappropriate for cases, such as this, in which the radioactive material is deposited in only one specific spot/location at the top of the SZ.*

Response: Sensitivity studies in the SZ have shown that the minimum size for the source term at the top of the SZ is approximately 100 m. Below this size, the resultant concentrations do not change at the 20-km boundary. For the potential SR and LA, elements at the water table in the SZ model will be approximately 100 m or less.

Comment 143 (pages 116–117): *The model developed for the SZ analysis is based on the assumption that the radioactive material is distributed over a wide area at the top of the SZ. This model, which then allows for estimates to be made of the downgradient transportation of the dispersed source, simply cannot be correct for application to the human-intrusion case. Although the TSPA staff recognizes this error, the net result is that the outcomes of the human-intrusion analysis are invalidated and the accompanying results are not meaningful.*

Response: As noted in the panel's comment, the M&O recognizes the limitations of these models. If future analyses of human intrusion require calculations of radionuclide transport from point sources, the models will be correctly developed.

Comment 144 (page 118): *The panel also believes that additional insight into the effects of climate change on repository performance could be gained by performing a sensitivity analysis in which the change to a glaciation regime is assumed to occur rather soon (say, within a few centuries) after closure, and to persist thereafter for about 100,000 years (which, on the basis of the historical climate record, is the typical duration for such glacial periods). Performing the entire TSPA analysis under such long-term-average climate conditions could help to illuminate several key issues related to repository performance.*

Response: Such an analysis was performed for TSPA-VA (DOE 1998a). The results of the expected-value base case (with climate change) are similar to the results of an analysis using only a long-term-average climate. One difference is that radionuclides released from a juvenile-failure waste package reach the accessible environment sooner when only the long-term-average climate is considered (about 2,000 years versus about 3,500 years). For the time period between 5,000 and 100,000 years, the dose rate is virtually identical for the expected-value base case and the case that only uses a long-term-average climate. This is because all of the waste packages that fail by corrosion do not fail in the expected-value base case until after the long-term-average climate occurs. Thus, the environmental conditions are similar in the two cases. The probabilistic base-case calculations for TSPA-VA (DOE 1998a) did have containers failing by corrosion as early as 3,000 years; for a long-term-average-only climate, more failures could be expected because more packages would be dripped on, and releases from these packages would reach the accessible environment sooner than for the base case.

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4. SPECIFIC COMMENTS ON SUB-SYSTEM MODELS OF NEAR-FIELD GEOCHEMICAL ENVIRONMENTS

4.1 MODELS OF INCOMING GAS, WATER, AND COLLOIDS

Comment 145 (page 120): *...the conceptual and parametric uncertainties associated with gas flow and composition are large; this is critical, as the CO_2-concentrations have important effects on solution composition and actinide mobilities.*

Response: The M&O agrees that the CO_2 compositions play a large role in the system chemistry. This was the basis for trying to incorporate the major sources of variation to this parameter in the TSPA-VA (DOE 1998a). The use of 1,000 ppmv (parts per million by volume) for ambient CO_2 is not arbitrary, but is the average of site measurements (see Figure 4-5 and Section 4.2.1.1.1 in Chapter 4 of the TSPA-VA TBD, CRWMS M&O 1998). This is taken to represent the ambient pore gas (i.e., the "air" in the rock) in the system and the potential effects on this system from thermal-chemical effects are evaluated successively on this value. These perturbations include thermal effects using both (a) the effect of dilution of the "air" by H_2O generation that is calculated in TH process models, and (b) chemical reaction in the host rock system including the degassing of CO_2 from heated water and the potential reaction of calcite to the released CO_2. The bases for these possible effects are process-level coupled THC models and the Single Heater Test results discussed in Section 4.2.1.2 and 4.2.3.1.1 of Chapter 4 of the TSPA-VA TBD (CRWMS M&O 1998). The changes for 200 years were calculated as an estimate of a highly uncertain time frame in a manner that shows up in the performance assessment time frame; the estimates represent a smeared, or averaged, gas composition over that time frame. Even with a high CO_2 value in "air," the value of the gas is low because it is swamped by the dilution effect for the abstracted 200-year period. If the 10 percent CO_2 in "air" is mapped to the process-level air-mass fraction (AMF) from the TH models, it reproduces, within an order of magnitude, the values of CO_2 being measured in the gas phase from the ongoing Drift-Scale Heater Tests. The isotopic composition of the CO_2 in those measurements also indicates that calcite is degassing CO_2, which supports the conceptual model used.

The effects that concrete may have on the CO_2 fugacity and dissolved carbonate are evaluated directly in the sensitivity studies on concrete that are analyzed in the TSPA-VA (DOE 1998a). However, the chemical effects of concrete are not included within the base case. The resulting fluid compositions from those concrete sensitivity studies directly reflect those effects on the CO_2 content and these were evaluated for their potential impacts to the waste package, the waste form, and radionuclide transport. Further development of coupled THC models will allow more detailed assessment of the changes in this system from these interactions. In addition, the LADS process has recommended an enhanced design with structural steel materials in the drifts instead of concrete to limit the possible impacts of the chemicals in the concrete on the mobilization and movement of radionuclides.

Comment 146 (page 120): *Panel notes and must emphasize that flow in the unsaturated zone and thermal-mechanical-hydrologic-chemical interactions must be closely correlated to incoming-water flux.*

Response: A work plan has been developed (for the TSPA-SR/LA) in the TH and coupled processes workshop to provide the water chemistry and gas-phase composition of the incoming water and gas at the scale of the emplacement drifts. This THC drift-scale model will include waste package heating and a specified subset of minerals and gas phase species (possibly based on the results of the Drift-Scale Heater Test). The drift-scale model will receive boundary conditions from the mountain-scale THC model for consistency.

Comment 147 (page 121): *We recommend that future model calculations utilize mineral-solubility constraints to determine the concentration of principal chemical components, such as Na^+ and K^+ as a function of temperature. Such calculations combined with experimental studies and models of mass transfer resulting from host rock-water interactions may reduce the present uncertainty in the compositions of the in-coming water.*

Response: The M&O agrees that mineral equilibria should be used where possible to constrain the concentrations of components within the geochemical calculations, and that was the intent of the settings used in the calculations. More detailed constraints on mineralogic controls on the water chemistry in this system should be developed to allow their implementation within these models of compositional evolution. Coupled THC models of the geosphere that include mineral-water-gas reactions should provide more comprehensive consideration of these mineralogic controls on the water chemistry in future analyses.

A fully coupled THC reactive-transport modeling capability is now available within the site-scale UZ flow and transport model. This modeling capability simulates temperature-dependent reactive chemistry among the components of an assemblage consisting of water, gas (CO_2 and O_2), and minerals, including silica, calcite, anhydrite, feldspar (K, Na, and Ca), smectite (Mg, Ca, Na, and K), kaolinite, illite, sepiolite and other sheet silicates. This modeling capability will be used to predict expected ranges of the chemical compositions of both water and gas entering potential waste-emplacement drifts during and after the thermal pulse. Additionally, this modeling capability is being tested by predicting the coupled THC effects expected to occur in the rock mass surrounding the Drift-Scale Heater Test in the ESF in advance of data collection.

Comment 148 (page 123): *During the period of boiling, a dryout zone will form around the repository. As the system cools, the boiling front and the outer boundary of the dryout zone will migrate back into the drift. As long as the outer boundary of the dryout zone is in the host rock, no water is expected to enter the drift. When water finally enters the drift, the arbitrarily chosen percentage of evaporated water (90 percent) may give rise to uncertainties in the modeled compositions.*

Response: The M&O agrees that the basis for this was unclear in the documentation. The choice of 90 percent evaporation was not arbitrary. It was chosen based on the results of a fully-coupled THC process-level model that showed that fluids in the vicinity of the drifts were about 10-fold more concentrated for conservative elements (Lichtner and Seth 1996). The model also showed that these would be candidates for the fluids entering the drift (see second paragraph of Section 4.2.3.2.2.4 in Chapter 4 of the TSPA-VA TBD, CRWMS M&O 1998). This discussion should have been included in other areas of Chapter 4 to clarify the choice of the 90 percent "boiled" fluid composition. Development of fully coupled THC models that will supply

a range of water compositions will allow a more explicit assessment of the uncertainty in the composition of the water entering a drift and provide transparent bases for the values used for future TSPA abstractions and analyses.

Comment 149 (page 123): *The abundance of incoming-colloids is assumed to be the same as that found in Yucca Mountain groundwaters as constrained by the ionic strength of the water. This relation is substantiated by the compilation of colloid concentrations in groundwaters of various ionic strengths from around the world... . Although this provides a basis for an estimate of colloid abundance, the estimate depends on the calculated values for the ionic strength of the water in the NFGE. The uncertainties in this estimate have already been discussed.*

Response: The M&O agrees that there are uncertainties associated with the specific fluid compositions that were used in the VA (DOE 1998b). However, because colloid concentrations are relatively insensitive throughout the range of these lower ionic strength fluids, and their concentrations decrease at higher values, the uncertainties are expected to have little affect on this specific constraint. Future analyses will reexamine and update the relation for colloid stability as function of water composition. A range of bounding fluid compositions will be used explicitly to evaluate the uncertainties involved here.

Comment 150 (page 123): *Additionally, the site-specific measurements and the global compilations may not be relevant to a repository that has experienced an extended thermal period.*

Response: The M&O agrees that thermal effects in the NFE will affect the geochemical conditions there, and that these changes will affect colloid stability and abundance in the incoming waters. To date, there is no clear way to address what these changes might be. Preliminary data from the Single Heater and the Drift-Scale Heater Tests indicated changes in local geochemical conditions in the host rock fracture-lining minerals and the ambient water chemistries.

Comment 151 (page 123): *Finally, the concentration of incoming-colloids may be affected by chemical reactions and colloid formation due specifically to materials present in the drifts (i.e., concrete, waste package containers and waste forms).*

Response: The M&O agrees that the specific measurements of colloid abundances would not apply to perturbed conditions. A functional relation is used to extrapolate the values for the calculated conditions, which are actually within the values measured. During the high-temperature conditions, fluids are expected to be controlled by the evaporative concentration of salts and be at higher ionic strengths that favor low concentrations of colloids. These values are expected to bound those conditions. Colloids generated by materials within the drift are represented by the In-Drift Colloids model, which takes the incoming colloids as input to it. The focus for TSPA-VA (DOE 1998a) was on the iron oxyhydroxy colloids, and additionally, two waste-form colloids that may be generated within the drift (Section 4.4.3.3 and 4.5.2.3 in Chapter 4 of the TSPA-VA TBD, CRWMS M&O 1998). The M&O agrees that additional supporting data for the conceptual model that the colloid stability limits the abundance of colloids suspended in the fluid, regardless of source, would be useful. Given the relations for the compositional dependence of colloid abundance, the water chemistry in the drift should be

usable to assess the resultant concentrations. As noted in the response to Comment 145, the LADS process has recommended design changes that limit the use of concrete in the potential repository. This design change would decrease the potential for generating colloids from cementitious materials in the system over the same period of time.

4.2 MODELING OF IN-DRIFT GAS

Comment 152 (page 123): *A primary issue is whether the models used in the sensitivity analysis (separate from the base case calculation) have the necessary scientific and technical basis to serve as an acceptable guide for the behavior of the system described by the base case calculation.*

Response: The two areas of investigation for changes in gas composition by reaction with the materials in the drift focused on assessing the potential changes to O_2 and CO_2 compositions in a bounding manner (Sections 4.4.3.1 and 4.6.2.1 in Chapter 4 of the TSPA-VA TBD, CRWMS M&O 1998). The analyses utilize basic mass balance comparisons of the base-case gas compositions and fluxes of O_2 and CO_2, with the major sink terms that were identified within the design for these constituents. In the case of oxygen, there is very little potential for changes based on the oxidation of metals, as 450 percent of the O_2 needed to oxidize all the waste packages is fluxed through the drifts in 4,000 years. This represents a far greater rate of oxygen use than is represented by the slow corrosion of package material and, therefore, is clearly untenable. For CO_2, the mass balance with cement as a sink indicated that it would be a potentially effective sink for CO_2 for at least 10,000 years (only 20 percent of the CO_2 needed for full carbonation). Therefore, the sensitivity studies for concrete reactions included explicit evaluation of the changes to CO_2 fugacities in analyses that are completely consistent with the base-case analyses. These are more uncertain because of the greater level of uncertainty in evaluating the cementitious system. However, the level of uncertainty in the calculations is not as large as having no evaluation at all of this alternate conceptual model of the system. As noted in previous responses, the proposed LADS design limits the use of concrete in the repository. This will reduce the potential for chemicals in the cement to affect the system over the same period of time.

Comment 153 (page 124) *In the absence of back-fill, there will be a large volume of atmospheric air remaining in the drifts at the time of repository closure. In this early period after the closure of the drift, the in-drift gas composition will be determined by the mixing of the left-in-drift atmospheric air and the incoming gas. We estimate that the initial amount of left-in-drift O_2 and CO_2 will be equal to the cumulative fluxes of these gases for the first several hundred years. Thus, variations in the estimate of the flux can have a substantial effect on the estimated compositions of the in-drift gas.*

Response: The TH calculations include evaluation of the air in the system at the start mixing with the H_2O generated during boiling. Thus, this mass should already be included within the material that is analyzed. Even if it is not, the masses involved in the first time period of 200 years, for TSPA-VA (DOE 1998a), would be off by perhaps a factor of two. That could lead to a change in the fugacities of a factor of two—which is still small compared to the dilution effect that is dominant during that time. The M&O agrees that, for detailed process models, ensuring that the initial mass is specifically accounted for is necessary. However, for abstracted

performance assessment models that average compositional effects over hundreds of years, this is not as important. For example, the fixation of CO_2 in cement during the preclosure period may be a much larger effect because it covers about 100 years. In addition, almost all of the CO_2 evaluated in the system for TSPA-VA (DOE 1998a) comes from water fluxing near the drift in the 5,000- to 100,000-year time frame, as opposed to direct gas flux through the drift. The proposed design changes from LADS include backfill in the drifts and more closely spaced waste packages. This design would minimize this issue, even for the detailed process-level models.

Comment 154 (page 124): *...we note that not all of the incoming gas will remain in drift or be consumed by in-drift reactions. The cumulative outgoing flux of each constituent gas in the drift should also be taken into account in order to determine the in-drift gas fugacities.*

Response: The air flux through the drift is given by the TH process model calculations, as are the AMF and the H_2O content of the gas phase, which is 1 minus the AMF (see Sections 4.4.2.1 of Chapter 4 of the TSPA-VA TBD, CRWMS M&O 1998). For the Incoming Gas model, the fugacities are handled by combining the AMF with the defined composition values of that air for O_2, CO_2, and N_2. Values for the incoming CO_2 gas represent geochemical reaction considerations in addition to the thermally driven dilution of the AMF. In consideration of changes to the fugacities resulting from reactions within the drift, the gas constituents are made available based on their supply rates to the drift at the fugacities given by the Incoming Gas model. During the thermal perturbation, these fugacities are already greatly decreased by the dilution effect constrained by the TH models. In order to assess additional first-order effects on O_2 and CO_2 for the abstracted time periods used in the NFGE performance assessment models, the cumulative gas flux was compared via mass balance to the major O_2 or CO_2 sinks. The calculations for the concrete sensitivity study were focussed on identifying the earliest point in time at which enough CO_2 had moved through the drifts to fully carbonate the reacting cement. This assumes that the calcite formation reaction is rapid, and not rate limiting, based on the observations of cements in the surface environment. Therefore, these sensitivity studies go out further in time (to the endpoints of each time period), and reacting the potential cumulative flux of CO_2 at that point in time with the initial concrete mass. If the calculation shows that the CO_2 "reservoir" is exceeded during that period, the CO_2 fugacity is allowed to change from the reaction and the resultant fluid chemistry is set by that composition. If this is not the case, the CO_2 fugacity does not change and the remaining is not reacted. These analyses ignore potential sources of CO_2, with microbial activity being the primary possibility. This potential however, was evaluated in the bounding calculations on microbial growth that resulted in masses that are too small to affect the bulk chemistry in this system. The recommended LADS design will limit the potential for chemicals in the cement to affect the system.

4.3 MODELING OF IN-DRIFT WATER/SOLID CHEMISTRY

Comment 155 (pages 124–125): *...Because the reaction rates of the minerals in the aggregate are much lower than those for the minerals in the cement, the change in water chemistry is considered to be controlled mainly by cement/water reaction. The main sources of uncertainty in this approach include:*

1. *The proposed mineral assemblage for cement is probably not typical of the cement after the thermal period. Elevated temperatures over an extended period may have a*

considerable effect on the concrete, e.g., carbonation. Thus, there is uncertainty in the mineral compositions that are obtained by cement phase normalization calculations based on the chemical composition of the cement.

Response: The M&O agrees that the evolution of the mineral assemblage within the cement system is an area of large uncertainty and that models for the evolution of those phases driven by the thermal and gas chemistry expected in the system would improve the NFGE models. This aspect is discussed in Section 4.7.3 of Chapter 4 of the TSPA-VA TBD (CRWMS M&O 1998). The thermochemical calculations performed included data on some of the possible phases, but this area is one for which comprehensive thermochemical data are not currently available. It is possible that the formation of more stable calcium silicate phases during the thermal perturbation would lead to fewer effects on the pH of the system. It is important that any model evolution of such mineral assemblages be defined for the appropriate controlling variable conditions that are expected to occur through time in the system. As noted in the response to Comment 151, there would be less potential for generating colloids from cementitious materials in the system over the same period of time with the recommended LADS design.

2. *The available solubility data for cement phases are generally limited to 25° C; thus, there is only a limited basis for extrapolating this behavior to higher temperatures.*

Response: The M&O agrees that the thermochemical data set (both equilibrium data and kinetic data) for cement phases is very limited, especially for higher temperature conditions. These uncertainties/limitations are discussed in Section 4.7.3 of Chapter 4 of the TSPA-VA TBD (CRWMS M&O 1998). This area of uncertainty could be addressed by synthesis of the existing data, experimental studies to measure key thermochemical values, experimental studies of phase stabilities at appropriate conditions, and by the restriction of cement usage to negligible quantities in the potential repository design.

3. *There are large uncertainties in the relative dissolution rates among the phases considered in the concrete (including cement and aggregate). The relative reaction rates of the phases in concrete were chosen based on the "observed" phase dissolution sequences. The sequence of relative reaction rates may be correct, but the actual values may be incorrect.*

Response: The M&O agrees that the actual reaction rates are uncertain for these phases. However, for the calculations performed, it is the relative rates that are the key for the resulting water compositions, etc., primarily because these analyses allow the reaction progress to go to large values (i.e., about 1). In the sensitivity analyses completed for the reaction of concrete (Section 4.6.2.2.1.2 of Chapter 4 of the TSPA-VA TBD, CRWMS M&O 1998), the relative reaction rates for the phases were varied in two ways: 1) they were all multiplied by factors of 0.2 and 5.0, and 2) they were set to equivalent values of 1.0 and 0.1. The results showed that the absolute magnitude of the relative rates had little effect on the results, whereas the results for equivalent rates were very different. The relative rates were chosen by ensuring that they reproduced the observed water chemistry resulting from the reaction with concrete. This area of uncertainty is more important for systems that are fast flowing (i.e., fracture flow pathways), where fluid cannot continue far in the reaction progress prior to advecting away from the mineral assemblages. See, also, the responses to Comments 151 and 155.3.

4. *In the calculation, the reactions are assumed to proceed to equilibrium depending on the relative magnitude of gas sinks apparently versus gas fluxes into the drift. Thus, reactions are considered to proceed until gas component reactants are unavailable in the drift. This assumption in the calculation may overestimate the reaction progress.*

Response: The M&O agrees that the assumption of the approach to near equilibrium may overestimate the reaction progress in an actual repository system. However, for concrete that is continuously being mechanically broken apart in a low water-flow system (assumed to occur in the base-case VA design [DOE 1998b]), this is the most appropriate scenario to analyze. The calculations were performed such that the reaction terminates at a value of 1 for the reaction progress, which corresponds to allowing a particular amount of solids to react with 1 kg of water. This reaction progress is sufficient to allow the system to evolve to a rock/solids dominated solution composition, although this may not represent an actual equilibrium system (i.e., the phases being added are not stable at the conditions of the analysis). The available gas reservoir is scaled as the solids are reacted within the calculations to assess whether or not it would be consumed during that period of time. This is the case for CO_2 in the first five time periods evaluating the concrete reaction, but in the sixth time period, the CO_2 reservoir is not completely depleted.

The oxygen contents of the gas were not analyzed in this manner because simple mass balance showed that there was plenty of O_2 available to oxidize the entire mass of the waste package within 4,000 years, assuming that the alloys could oxidize as fast as the O_2 was supplied. This is a very high rate, but it would be necessary to utilize virtually all of the supplied O_2 (i.e., 99 percent) in order to shift the fugacity by two orders of magnitude. This bounding analysis indicated that O_2 will only be low during the active boiling period, where it is already reduced by the TH air dilution effect, and that no long-term reducing environment can be expected within the drifts. Because the waste package corrosion models do not have any corrosion occurring in the above-boiling condition, there was little push to further define additional O_2 depletion during this period via waste package corrosion. Further decreasing the O_2 fugacity values at the waste form surface during this period would be misleading unless radiolysis were also included. However, if similar calculations were performed for O_2 reactions using the corrosion rates to supply the reacting alloy masses, the small O_2 reservoirs would be exceeded during the first two time periods, but for all other periods, the O_2 reservoirs would not be completely exhausted. The alloys for the waste packages and drip shield in the proposed LADS design are expected to have even lower corrosion rates and, as such, are expected to have even less effect on oxygen in the drift.

Comment 156 (page 125): *There are many conceptual and parameter uncertainties in the model implementation. These uncertainties include: 1.) the extent to which the seepage flux actually passes through the spent fuel is uncertain; 2.) the extent to which the alteration products protect the spent fuel from further dissolution was not considered in the model; 3.) the percentage of spent fuel and the actual surface area that would be exposed and subject to dissolution is uncertain (this depends directly on assumptions made concerning the durability of the cladding and the evolution of the surface area of the UO_2 as corrosion proceeds); 4.) the rate constants for dissolution and precipitation are not known; 5.) the thermodynamic data for the uranyl phases that form on alteration are limited and in some cases contradictory... .*

Response: As uncertainties always exist, bounding analyses were conducted wherever possible, as suggested by the Panel. For example, the protective effect of the alteration products on the spent fuel by inhibiting further dissolution lacks experimental support and is difficult to quantify; however, by omitting it, the fuel is maximally exposed to dripping water. Therefore, the dissolution of fuel, the radionuclide release, and the modification of the water chemistry are conservatively bounded.

The M&O does not agree with the general assessment that "the rate constants for dissolution and precipitation are not known." In fact, the rate constants for schoepite, soddyite, and uranophane are derived from the Swedish Nuclear Fuel and Waste Management Co. experiments (Casas et al. 1994; Bruno et al. 1995; Perez et al. 1997; Casas et al. 1997). The M&O agrees that there is room to improve the experiments; nonetheless, they are known parameters with some degree of uncertainty, and the effects of that uncertainty on the final modeled results will be evaluated.

It is natural that the thermodynamic data of uranyl minerals change over time. As more and more is learned about the uranyl minerals, and the experimental methods improve, the quality of the thermodynamic data also improves. The M&O is reviewing the thermodynamic data of uranyl minerals. As the modeled results match the observations from the drip tests and the Peña Blanca natural analogue so well, the M&O believes that the quality of the data used for the simulations is reasonably good.

Comment 157 (pages 125–126): *In the sensitivity analysis, different water flux scenarios through the waste package and different thermal-chemical kinetic databases and constraints demonstrated that the bulk composition of the fluid was not sensitive to the corrosion conditions and dissolution rates of spent fuel. In the absence of supporting experimental data, this is a questionable conclusion. This is a good example of the use of a sensitivity analysis in place of experiments.*

Response: The M&O agrees that this phenomenon calls for a more detailed examination. There could be several reasons, one of which could be that the system itself has a certain buffering capability and the range of changes is within this capability. It could also be an artifact, and this possibility was not excluded from consideration.

Comment 158 (page 126): *The discussion of the near-field environment should summarize the potential impacts of the radiation-field and explain the extent to which such phenomena are considered relevant to models used in TSPA.*

Response: The M&O has considered the impacts of the radiation field on the corrosion of the metallic barriers and the spent fuel. The radiation dose at the surface of the waste package was found to be well below the threshold for enhancement of corrosion of the outer metallic barrier. This effect is being re-evaluated for the LA designs.

The M&O agrees that the more detailed process-model analyses of the spent fuel reaction could be improved by including radiolysis effects. However, the current spent fuel dissolution rate model used in the TSPA is based on far-from-equilibrium forward dissolution rate studies under oxidizing conditions and is taken as a bounding model for this process. The effects of radiolysis

at the fuel surface is an area where models are being developed. These models will be included in the next TSPA, as appropriate. This would be particularly important if a more descriptive spent fuel evolution model were to be developed that potentially limited the alteration rate of the primary spent fuel.

Comment 159 (page 127): *The analysis of microbial activity in the near-field environment was judged by the Panel to be at a preliminary stage.*

Response: The M&O agrees that the In-Drift Microbial Model is a preliminary analysis, but it provides the first order of magnitude bounds on the potential abundance of the microbial population within the drift environment, as well as the basis on which the M&O can focus its efforts to address issues regarding microbes.

Comment 160 (page 127): *The Panel simply notes that the uncertainties in the modeled results are large and any conclusions based on the results are essentially speculative. This is due to the need by analysts to make some rather important underlying assumptions.*

Response: The M&O agrees that this area is one where uncertainties are relatively large. However, this model of microbial growth appears to give reasonable order-of-magnitude estimates. In fact, the analyses were performed for the natural system microbial population and the results compared, within about an order of magnitude, to the actual measurements. This was the case even though the uncertain biotite degradation parameter was varied from 1 million to 10 million years and variable infiltration rates were analyzed (Section 4.6.2.3.2.3 and Figure 4-83 of Chapter 4 of the TSPA-VA TBD, CRWMS M&O 1998). This agreement with independent measurements indicates that there is some degree of confidence that this model can be used for order-of-magnitude assessments. Additional comparisons will be made between model calculations and experimentally determined microbial growth rates to further assess the confidence that can be placed in this model.

Comment 161 (page 127): *The Panel concludes that this complex set of assumptions and information requirements used to analyze the contribution of microbial growth lead to a highly uncertain and speculative estimate.*

Response: The M&O agrees that there are uncertainties in these analyses, especially in the area of the material lifetimes. However, these analyses provide a systematic set of analyses with which to evaluate and prioritize the potential effect that gives a first order of magnitude estimate for the growth of microbes in this complex system. These analyses were performed for a range of possible material lifetimes for the key nutrient or energy source materials in order to assess the magnitude of those uncertainties. The bounding estimate of microbial growth from these analyses was utilized. This represents an improved basis for focusing the M&O's efforts to address these issues over the previous situation in which the potential abundances of microbes in the system were unbounded.

Comment 162 (page 127): *Taken as a whole, the Panel does not see the above approach as a clear path to answer the concerns regarding microbial activity. The answers to these questions are not likely to come from more sophisticated models and analysis, which require unavailable*

information, but rather from bounding analysis and the selection of materials which resist microbial activity.

Response: The model employed, although complex, is relatively simple in other aspects and evaluates, in a systematic fashion, the same information a person would need to assess in order to make the selection of materials suggested above. As stated above, the M&O considers this model to be a useful tool for order-of-magnitude assessments of the microbial abundances and which simultaneously assesses the potential contributors to that growth and identifies the potential limiting materials.

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