FINAL REPORT

TOTAL SYSTEM PERFORMANCE ASSESSMENT

PEER REVIEW PANEL

February 11, 1999

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Peer Review of the
Total System Performance Assessment-Viability Assessment

Final Report

February, 1999

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PREFACE

From its inception, the Peer Review Panel has been aware of the difficult task facing the TSPA-VA staff in the analysis and evaluation of Yucca Mountain as a site for a repository for radioactive waste. Modeling the probable behavior of the proposed repository requires the characterization of a complex geologic setting and detailed analyses of a complicated and, in many ways, unprecedented set of problems.

As set forth in the Peer Review Plan, the Panel's mission in this final report was to review the completed TSPA-VA and to provide comments, concerns, conclusions, and recommendations that could be used in the development of a TSPA to support a license application, if the project progresses to this stage. In this regard, it is important to note that the Panel has reached no conclusions as to whether the TSPA-VA demonstrates that the proposed repository is acceptable or whether the project staff should proceed to the licensing application phase. This was not within our charge. All comments and recommendations in this report should be considered with this view in mind.

In seeking to meet its assigned mission, members of the Panel have taken it to be their responsibility to identify problems and weaknesses in the approaches used and in the analyses conducted by the TSPA-VA staff. The primary goal of this effort was to assist the staff in focusing on those improvements crucial to the development of the TSPA, before it undergoes the critical review inherent in any type of licensing process. Because of the analytical and modeling difficulties noted by the Panel and the serious manner in which we viewed our assignment, this final report can be interpreted as being highly critical of many aspects of the TSPA-VA. While this may be the case, the Panel wants to emphasize that its criticisms are submitted solely with the objective of providing suggestions and recommendations that will be constructive and will help move the TSPA process forward. Panel members encourage those who disagree with its findings and recommendations to engage in discussions with one another and the Panel to clarify these disagreements and advance the understanding of all participating parties.

The Panel expresses its appreciation to the TSPA staff and other scientists and engineers working on the project for all the assistance that they have given us. The TSPA-VA is a comprehensive and complex analysis, and we frequently found it helpful to talk to project staff to confirm our understanding of how the analysis was being done. In such cases, we always found the staff to be responsive and cooperative. We would thank each of these people by name were it not inevitable that we would leave out one or more individuals who assisted.

We also thank Susan Wiltshire and Yanis Yortsos for their contributions. As the Panel's technical secretary, Susan has managed the details of assembling numerous versions of documents coming from the Panelists into a complete report, and has provided the Panel with thoughtful reviews of draft report sections that focus on both the overall objectives and findings of the review as well as with the specifics of how the findings are to be communicated. Yanis Yortsos, Professor of Chemical Engineering at the University of Southern California, has been a consultant to the Panel in the areas of thermal hydrology, unsaturated zone flow, and unsaturated and saturated zone transport. During the time that this final report was written, Yanis has essentially acted as a member of the Panel, taking the lead on specific technical issues, drafting our findings, and participating in the discussions that make this final report truly a team effort. The Panel also thanks Fanrong Chen of the University of Michigan and Mickey Hunacek and Cheryl Smith of Dade Moeller & Associates, Inc. for their assistance during this study.

Finally, we thank Tom Rodgers for all his assistance as our point of contact with the project's Managing and Operating Contractor. It has been a pleasure for all members of the Panel to work with Tom because he has handled all our organizational and administrative activities with great competence and efficiency, enabling us to concentrate on our review.

CONTENTS

LIST OF FIGURES

EXECUTIVE SUMMARY

A. Introduction

The TSPA-VA Peer Review Panel (the Panel) was formed to provide the Civilian Radioactive Waste Management System Management and Operating Contractor (CRWMS M&O) with a formal, independent evaluation and critique of the Total System Performance Assessment - Viability Assessment (TSPA-VA) for the proposed high-level waste repository at Yucca Mountain. The objectives of the Panel were to describe the technical strengths and weaknesses of the TSPA-VA and to provide suggestions for its improvement, as the TSPA staff moves ahead to prepare documentation in support of a possible license application (LA).

The Panel issued three interim reports prior to the completion of the TSPA-VA. These were based on draft documents supplemented by formal and informal meetings and interactions with the TSPA-VA staff. The comments in this final report were based on documented work, namely, the completed TSPA-VA (CRWMS M&O, 1998d) and its supporting Technical Basis Documents (CRWMS M&O, 1998c) and on other documents cited as references to this report.

B. Key Findings

The objective that Congress defined for the TSPA-VA was to assess "the probable behavior of the repository." Judged on that basis, the Panel finds that a number of the components of the TSPA-VA analysis were not supported by adequate evidence that they 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, as described in this report. For these reasons, it is unlikely that the TSPA-VA, taken as a whole, describes the long-term probable behavior of the proposed repository. In recognition of its limitations, decisions based on the TSPA-VA should be made cautiously.

With the benefit of hindsight, the Panel finds that, at the present time, an assessment of the future probable behavior of the proposed repository may be beyond the analytical capabilities of any scientific and engineering team. This is due to the complexity of the system and the nature of the data that now exist or that could be obtained within a 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.

The TSPA-VA was a necessary and useful step in the evolving understanding of how a repository could be expected to perform at Yucca Mountain. It has produced valuable insights into the performance of various repository components, and has helped identify issues where additional data and analyses could lead to improved understanding of the repository's performance. It has also been useful in identifying aspects that are comparatively unimportant to performance, for which additional data and analyses are not likely to be beneficial.

The Panel recognizes that substantial amounts of field and experimental data have been developed in support of the TSPA-VA; however, many elements of the analysis require additional data to be credible. These 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. While it obviously is not feasible to test the full TSPA-VA, it is feasible to test many of the individual component models experimentally. We note that many experiments are planned or in progress that should be useful in confirming, calibrating, or invalidating models developed for, or applied to, analyses of conditions at the proposed repository. Sensitivity analyses, although of value, cannot substitute for such experiments, because the sensitivity analyses used in the TSPA-VA often do not directly address the uncertainties associated with the experimental database or the selection of a conceptual model.

To be credible, it would have been necessary for the TSPA-VA to have included: (1) component subsystem models that capture the important and relevant phenomena; (2) databases that are adequate and substantially complete, where possible; (3) a proper and demonstrable description of the coupling between the subsystem models; and (4) adequate tests and evaluations of the modeled behavior. Although the TSPA-VA offers many examples of partial, even substantial, success in each of these four areas, the Panel observed examples of important deficiencies in each. Concerning items (1) and (2), the final positive estimates of performance described in 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, the performance of the cladding and the waste package. Concerning item (3), the Panel believes that it may be beyond the capabilities of current analytical methodologies to analyze systems of such complexity and covering such spatial and temporal scales. For this reason, we believe that the effects of coupled processes can best be dealt with through a combination of bounding analyses and engineered features designed to minimize the effects of such processes. Concerning item (4), the TSPA-VA does not contain the convincing direct measurements or confirmation of the modeled behavior of components or subsystems even where such testing is feasible. This type of testing should be a part of the analysis of such a complicated system.

As noted above, the assigned 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 will comply with the applicable regulatory limits. These are significantly different objectives, and recognition of this distinction should be an important element of the path forward to the TSPA-LA. This issue is discussed in more detail in Section III.

C. TSPA-VA Methodology

On the basis of its review, the Panel concluded that certain portions of the TSPA-VA were well done; the Panel also concluded that serious questions remain as to the adequacy and acceptability of other portions of the analyses. On the positive side, the Panel noted that the overall performance assessment framework and the approach used in developing the TSPA-VA were sound and followed accepted methods. The Panel also observed that certain of the technical complexities and uncertainties associated with the analysis were unusual, if not unique. Prominent among these were the unprecedented time periods over which the performance of the proposed repository is to be assessed; the heterogeneity of the site; the multitude of the paths through which radionuclides could be transported and ultimately come into contact with offsite groups; and the complexity of the processes that interact to affect hydrological and chemical conditions within the proposed repository and its environment.

The Panel readily acknowledges that many of these technical complexities are difficult to analyze. In general, such a complex analysis may incorporate significant errors if the wrong deterministic model for specific phenomena is selected, or if an incorrect analytical solution for the model or an incomplete description of the system to be modeled is used. For the TSPA-VA analysis, the evolution of groundwater compositions over time is especially difficult to estimate, as are the phase assemblages formed during the alteration and weathering of spent fuel. Another complicating factor is that several groups of phenomena within the proposed repository involve complex coupled processes. These include phenomena in the unsaturated zone above and near the repository that govern the environment surrounding the waste packages; phenomena that control waste degradation inside the packages after package degradation has begun; and the behavior of radionuclides in the unsaturated zone and saturated zone environments. Sufficiently detailed coupled models have not been developed in the TSPA-VA to permit an integrated analysis to be performed in either of the first two cases.

The lack of an adequate theoretical basis for certain of the models was a major contributor to the analytical difficulties in the TSPA-VA. Exacerbating the problem was a lack of sufficient site-specific data to evaluate and confirm the models. Although in some cases, this lack was confirmed by independent reviews by Panel members, in other cases these efforts showed that additional data existed that could have been used. An important point to recognize is that in such circumstances, elicited expert opinion should not be used as a first option for filling such needs. If data can be obtained through measurements in the laboratory or field, in a reasonable time and at a reasonable cost, this should always be the preferred approach Because of the inherent complexity of the proposed repository and the number of phenomena that need to be analyzed, the TSPA-VA analysts used a simplified form of the detailed process-level models to reduce the associated computational requirements. These simplified models were referred to as model abstractions. The Panel agrees that this approach is sound in principle. However, some issues remain, such as the exact basis for the abstracted models. An abstraction should be a simplification of a more fundamental process-based model, and it should provide results consistent with such models over the same range of parameter and input values that can be taken into consideration in the more complicated approach.

D. Future Actions to Improve the TSPA

As the Panel has observed in its review, the objectives for the TSPA-LA differ significantly from those for the TSPA-VA. Recognition of this distinction should be an important element of the path forward to the TSPA-LA.

For cases in which it is feasible to improve either the component models or their underlying data, the Panel recommends that primary attention be directed to those changes that will affect the overall assessment of the proposed repository. Where conservative bounding analyses do not result in an unduly pessimistic estimate of total system performance, it may not be cost-effective to refine the assessment in an attempt to make it more realistic. For those systems and events for which, by virtue of their complexity, it is not feasible to produce realistic models supported by data, the Panel recommends that, if possible, a combination of bounding analyses and design changes be applied.

There are some aspects of the analysis for which additional data collection and modeling will produce only small reductions in uncertainty. If certain aspects of the complex coupled phenomena can be ignored or treated one-dimensionally, the overall analysis will be vastly simplified. At the same time, however, care is needed to ensure that the use of bounding analyses does not result in unacceptably conservative projections of the performance of the proposed repository. In such cases, we recommend that, where it is possible, the project staff demonstrate, either in the TSPA-VA reference design or in a revised design, that a specific group of uncertainties have only limited consequences with respect to the overall repository performance.

Although the Panel cannot predict what will be necessary if the project reaches the stage of submitting a licensing application, it is almost certain that the U.S. Nuclear Regulatory Commission will require a documented understanding of the underlying processes, assumptions, and analyses that goes well beyond that which was presented in the TSPA-VA. To accomplish these goals and to achieve the required degree of confidence, the Panel recommends that the project staff begin in its future efforts with a simpler set of analyses, and then evaluate the more complex issues through either sensitivity studies or bounding evaluations.

Since the projection of the performance of the proposed repository by the TSPA-VA is conditioned largely on the effectiveness of the waste package and cladding, particular attention needs to be directed to these components of the proposed barrier system. Important examples of key issues include the possibilities that the buildup of corrosion products from the outer carbon steel layer could cause early failure of the inner corrosion-resistant layer of the waste packages, and that the credit taken for spent fuel cladding may be optimistic, considering the potential effects of hydrogen embrittlement. Although the TSPA-VA contains many useful sensitivity analyses that illuminate the behavior of certain components and systems within the proposed repository, those analyses taken as a whole do not provide sufficient insights to overcome these deficiencies and uncertainties. Where such analyses produce results that are inconsistent with intuitive judgments, the underlying models and parameters should be examined to ensure that uncertainties in the performance of the proposed repository are appropriately represented.

E. Specific Technical Observations and Findings

Advances and Improvements in the TSPA-VA Analysis

The TSPA-VA contains many substantial advances and improvements over earlier similar reports. Perhaps the most dramatic change has been in the approach used to assess the rate of infiltration of water into the mountain. On the basis of this change, the maximum assumed rate has been revised upwards by an order of magnitude. This is consistent with the recent discovery of fast flow paths within the site, as evidenced by the findings of the ^{36}Cl studies. One direct result of the use of this refined analysis is a shift in the project team's concept of the way flow and transport occurs from predominantly matrix flow-dominated regimes to fracture flow-dominated regimes. The revised interpretation of infiltration has also led to a more realistic representation of the fracture-matrix interaction, although it is still far from complete, and to an improved characterization of the hydrologic properties of the geologic setting. Another significant development was the incorporation, for the first time, of a model for analyzing seepage in the drifts. The hydrology of the near-field environment is now modeled at a much smaller scale. Outcomes of the Drift Scale Test and related investigations in the engineered barrier system will be useful in testing these models.

The project team has also 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. This model is not physically representative of the saturated zone transport for isolated waste package failures. Nonetheless, sensitivity analyses indicate it overestimates dilution for such cases by perhaps a factor of three. If this is accepted as being an indication of the actual situation, this factor is small in comparison to the other uncertainties in the saturated zone assessment.

The TSPA-VA staff has made a concerted effort to study the complex interaction problems resulting from the thermal pulse, as described in the published literature. Of particular significance are the analyses of coupled thermohydrological, thermochemical, and thermomechanical effects. The work on thermal hydrology has progressed significantly since the TSPA-95, but work on thermochemical effects is still lacking. The staff is now linking hydrology at the drift scale to processes at the site scale, at least during the thermal period, and to thermohydrological, thermochemical, and thermomechanical processes. Also worthy of note are published results of sensitivity analysis of the saturated zone; the introduction of geostatistics for assessing flow, transport and retardation in the unsaturated zone; and the analyses of the various tests currently under way, including the single heater test, the large block test, and the drift scale test.

Key Role of Infiltration and Seeps Analysis

According to the TSPA-VA, "limited water contacting waste packages" is one of the four basic attributes of the proposed repository. Infiltration and seepage into the drifts are the main factors controlling such contact. Within the TSPA-VA, the seepage rates and the corresponding fraction of packages that are wetted were determined from a random sampling of a response surface obtained from a detailed analysis of the seepage into an individual drift. This probabilistic approach reflects the uncertainty in the capillary and flow properties of the fractures at the drift scale. The percolation flux is a direct reflection of the average infiltration flux above the repository.

The approach used in the analysis of seepage into the drifts, which the Panel considers to be both novel and informative, was based on an assumed steady-state flow in a fracture continuum, in which seepage commences where conditions exist for the drift surface to become fully saturated. A percolation flux threshold is estimated; below this threshold, seepage is assumed not to occur. However, because estimates of the percolation flux depend on the permeability and capillary structure of the fracture continuum in the immediate neighborhood of the drifts, these estimates are subject to the large uncertainty in the knowledge of the heterogeneity, spatial correlation, and anisotropy of these properties. During the period of the thermal pulse, thermomechanical and thermochemical effects may alter both the permeability and capillary structure of the fracture network and the seepage patterns as a function of time. This raises the possibility that seep locations will shift with time. The present analysis assumes that dry waste packages remain dry and wet packages remain wet as long as the climate remains constant. If, instead, the seep locations shift, more waste packages would be expected to experience liquid water, but with less frequency for some. During the dry periods, the corrosion rates would be reduced. The possible development of a precipitation cap may reduce the amount of seepage in drifts over which such a cap forms. It is not surprising, therefore, that the assessment of seepage and of the number of waste packages that will experience water drips is highly uncertain. For these reasons, it is not clear to the Panel that the present approach correctly captures the seepage behavior of an individual drift.

The large uncertainty in the seepage analysis is unfortunate, because seepage into the drifts is one of the most sensitive parameters in the dose estimates presented in the TSPA-VA. Given the uncertainties described above, the long term effect of the percolation rate on seepage cannot be calculated with a reasonable degree of accuracy. In addition, the percolation rate is itself uncertain due in part to uncertainties in long-term climate predictions.

Key Role of the Waste Package

Based on the TSPA-VA results, the TSPA analysts have judged that the rate of waste package degradation is a principal determinant of overall repository performance. The integrity of the waste package as a barrier is important to the performance of the repository as projected within the TSPA-VA for each of the time periods considered: 10,000, 100,000 and 1,000,000 years.

The waste package contributes to the containment strategy in two ways: first, it provides complete isolation until such time as the package is fully penetrated and, second, it provides subsequent retardation of the egress of radionuclides from the penetrated package. The Panel concluded that the conceptual description and analysis of the corrosion of waste packages are well underway and the needs are well defined. The Panel notes, however, that the understanding and treatment of how corrosion damage of a waste package evolves over time are not well developed. There is a need for improvements in the conceptual description, in the approach to the problem, and in the completion of the necessary experimental work. Once these improvements have been accomplished, the next step will be to complete the necessary analytical analyses.

The largest and most realistic threats to waste package performance are localized corrosion processes such as pitting, crevice corrosion, and stress corrosion cracking. Therefore, it is prudent and sound engineering practice to emphasize corrosion resistance in the design of the waste packages and in the selection of materials to be used in them. In general, the key issues and processes, as well as the corrosion performance of various candidate materials, are reasonably well understood. It is primarily the specifics in applying this knowledge to an analysis of the proposed repository, and the validation of this analysis with relevant data, that are still being developed and need further work.

The ambient waters at Yucca Mountain are innocuous to corrosion-resistant metals. From the standpoint of the proposed corrosion-resistant layer of the waste package, any chemical changes in these waters that occur as a result of thermal hydrological effects at the drift wall and in the surrounding rock are relatively unimportant; the waters will remain innocuous. What is important are the chemical changes that may occur through processes taking place at the waste package surface. This being the case, what needs to be determined and properly considered are any chemical changes that occur as the incoming water interacts within the engineered barrier system and, in particular, those changes that occur on or very near the waste package surfaces

Reactions at the metal surface, under deposits and in crevices will significantly change the water composition. Of most concern are metal-nonmetal crevices with corrosion products, deposits, rock and debris, and metal-metal crevices involving C-22/steel, C-22/C-22, and C-22/Ti.

The Panel identified several physical events and processes that affect the waste packages that were not considered or not sufficiently covered within the TSPA-VA. All of these are deemed to be important to the determination of waste package performance:

1. Expansion due to the formation of iron oxide corrosion products. The resulting expansion in volume (up to a factor of two) due to the corrosion of steel was not analyzed in the TSPA-VA. Such expansion can spall coatings and deform materials in contact with steel.

2. Treatment of waste package fabrication, transport, and emplacement. This adds to uncertainty. Procedures used in welding, heat-shrink fitting in assembling the canisters, in supporting the canisters on pedestals, and associated fabrication activities can have significant effects on corrosion and performance.

3. Corrosion processes in moist sand/particulate matter. After an initial period, waste packages are likely to be covered with particulate matter, e.g., intentional backfill, debris, and corrosion products, rather than remaining clean. Corrosion under these conditions was not evaluated within the TSPA-VA either through analysis or experiments. For steel, corrosion rates are likely to be significantly higher under these conditions, as contrasted to the situation for immersion. For corrosion-resistant metal, the effects on localized corrosion are uncertain.

4. Corrosion of steel beneath corrosion-resistant metal. For a waste package design with outer corrosion-resistant metal and inner steel barriers, the TSPA-VA analysis was likely highly conservative for steel, i.e., it overstated the corrosion rate.
5. Incomplete status of the analysis of stress corrosion cracking of C-22 and other Ni-Cr-Mo alloys. The performance of such alloys is a function of the corrosive environment, metallurgical condition, and tensile stress state. Further analysis and experimental data are needed in support of the assessments of these effects.

The Panel notes that there are insufficient data and analyses at this time to support fully or to discard any of the options being considered for a final waste package design. A rationale, backed up by analysis and data, is required for the specification of metals (both sequence and thickness) for the waste packages. The analyses for the TSPA-VA were performed using the waste package degradation (WAPDEG) model, which provided an understanding of the corrosion behavior of the waste packages. The analyses, however, were developed to a level of complexity that extended well beyond the data that were available. This complexity may be useful for the anticipated LA phase if sufficient data on key parameters become available. If not, the Panel believes that attempts to apply the WAPDEG model may compromise the transparency of the treatment. Necessary changes include an updating and/or revision of the model, including better integration of the multitude of process models used for analyzing various degradation modes or engineering enhancements, and the development of a more rational and stronger case to confirm the linkage between the process models and their abstractions.

At this time, the experimental data available to the TSPA staff are insufficient for determining (1) the performance of various alloys under anticipated conditions within the repository, and (2) the composition of the water that will interact with the waste packages. For this reason, the TSPA-VA staff depended to a large extent on expert elicitation. While these estimations were useful at this stage, the Panel concluded that significant improvements may be required for the anticipated TSPA-LA phase. The Panel also believes that it should be possible to resolve these deficiencies at reasonable cost and within a reasonable time.

Disruptive Events

The Panel reviewed five categories of events that could potentially disrupt the proposed repository. These were earthquakes, volcanism, criticality, human intrusion, and climate change. Highlights of our review are as follows:

Earthquakes

The primary seismic concerns were exemplified by various scenarios in which postulated rockfalls might damage a waste package. For other seismic effects, including flowfield disruption, effects of fault displacement, and groundwater-level rise, the TSPA-VA staff asserted with plausibility arguments that the impacts would be minor. The Panel concurs with these findings.

Volcanism

On the basis of extensive analyses of the direct-release volcano scenario, the information in the TSPA-VA concludes that this pathway is not an important contributor to doses to offsite population groups. The Panel concurs.

Criticality

Based on a detailed analysis of one specific spent-fuel in-canister scenario assumed to occur at 15,000 years, the TSPA-VA analysts estimated that potential criticalities were highly improbable and would, in any event, produce only modest increases in doses offsite. Other criticality scenarios appeared to be less likely than the in-canister scenario. The Panel finds these results to be reasonable.

Human Intrusion

It is assumed in the TSPA-VA analysis that an inadvertent intruder, in seeking to obtain groundwater, drills a single borehole at the repository site. The Panel concluded that the selected scenario is unrealistic, principally because of the extremely conservative assumption that all of the impacted waste goes downward to the saturated zone, rather than being pulled to the surface, and because of the potentially non-conservative modeling of transport in the saturated zone.

Climate Change

The effect of climate change on projections of repository performance is significant. However, predictions of climate change are difficult to make and impossible to confirm. Based on the existing state-of-knowledge, climate-change experts believe that the current interglacial period, which has lasted for several thousand years, will inevitably end. When this occurs the projected glaciation would probably not reach as far south as Yucca Mountain, based on past ice ages. Nonetheless, there would be substantial cooling and increased precipitation. The TSPA-VA projections are that the infiltration rate through Yucca Mountain will increase from the estimated present-day annual value of 7 mm to a long-term average of about 40 mm. This, as noted elsewhere in the report of the Panel, would have a pronounced effect on repository performance.

Overall, the Panel believes that the approach taken by the TSPA-VA staff to examine the future time at which a change in climate may occur is reasonable. Whether the accompanying analysis of the infiltration that would accompany an increase in precipitation is reasonable is less clear; the projections were disputed by a recently published review from the U.S. Geological Survey (USGS, 1998).

Potentially Non-Conservative Approaches

In the course of its review, the Panel identified several issues for which the assumptions made by the project staff in developing the TSPA-VA may be unduly optimistic. An example is the long-term performance of Zircaloy cladding on spent fuel. Another non-conservative assumption, used in the biosphere analysis, pertained to the buildup of radionuclides in soil irrigated with contaminated groundwater. Both of these issues are discussed in Sections II and IV of the Panel's final report. The soil buildup issue is summarized here to illustrate some of the concerns of the Panel.

Buildup of Radionuclides in Surface Soil

For calculation of doses that might be experienced after contaminated groundwater has reached the Amargosa Valley, it was assumed that residents pump water for consumption and for irrigation. With continuing irrigation, the concentrations in the soil would increase with time, eventually reaching a steady-state condition in which the annual additions to the soil will be equal to the annual losses. Losses of radionuclides from the soil can occur by wind or water erosion. Radionuclides can transfer to crops that are subsequently harvested, or weather down into the soil below the crop root zone. The effects of using contaminated groundwater were calculated using the GENII-S model, which permits the analysts to specify the length of time that irrigation water is deposited on the soil prior to the assumed period of intake. In the TSPA-VA model analyses, the time period for irrigation was assumed to be one year. If, in reality, some locations are irrigated for hundreds or thousands of years, the Panel has concluded that this assumption could lead to sizable underestimates of radionuclide concentrations in the soil, the amount depending on the particular radionuclide. Since the concentrations of radionuclides in plant roots depend on the concentrations in the soil, this will, in turn, lead to underestimates of the radionuclide uptake by root crops and to an underestimation of doses to exposed groups that consume these crops.

Data and Research Needs

Two types of data are needed: (1) fundamental data that are essential to the development and implementation of the models; and (2) data sets that are designed to challenge the conceptual models and to test the success of the coupled models. In developing the TSPA-VA, the project staff devoted considerable effort to meeting these needs, both through measurements in the field and experiments in the laboratory. The success of any future phases of the project, however, will depend on the continued direction of a substantial amount of effort to these needs. This will be especially important if more sophisticated models are incorporated into the analyses.

At the present time, there are several important areas in which the need for data has not been met. This is one of the reasons that a substantial part of the knowledge base in certain key areas presently rests on expert elicitations. Such areas include flow in the unsaturated zone, the near-field environment, waste package degradation, waste form degradation, radionuclide mobilization, and flow and transport in the saturated zone. In a similar manner, solubility limit distributions for several of the key radionuclides come from a limited experimental database; many are based on reanalysis of data from previous experiments. If there is any area amenable to experimental study, it should be the determination of concentration-limits in relevant solution compositions.

In addition, the experimental data needs associated with waste package design and assessment, noted above, include the determination of the critical temperature for alloy 22 in anticipated chemical environments and the measurement of corrosion rates of waste package materials and Zircaloy cladding when they are experiencing corrosive conditions.

An experimental program can advance the spent fuel corrosion model beyond its present empirical representation that is based on a regression analysis. Since over ninety percent of the radioactive waste that is intended to be disposed in the repository is spent fuel, a considerable knowledge of spent fuel corrosion is needed.

Although laboratory studies can serve as a source for some of these data, in other cases the needs can better be met through additional characterization of the site. In terms of the latter effort, there is a broad area along the projected saturated zone flow path from Fortymile Wash to the Amargosa Valley, 10 km or more in length, in which no boreholes have been drilled. In essence, site characterization has not been completed for over half of the projected length of the saturated zone flow path. The resulting voids include data on key subjects, such as subsurface geology, watertable configuration, and hydraulic parameters.

I. Introduction

This is the final report of the Total System Performance Assessment (TSPA) Peer Review Panel (the Panel). Although the Panel has prepared three interim reports, this final report is intended to stand alone. Hence, some of the recommendations and observations contained in the interim reports are repeated here.

A. Nature of TSPA Peer Review Process

In the Energy and Water Appropriations Act for fiscal year 1997, Congress specified four components of a viability assessment for a proposed high-level radioactive waste repository at Yucca Mountain, Nevada. One of these was to complete:

> ...a total system performance assessment, based upon the design concept and the scientific data and analysis available by September 30, 1998, describing the probable behavior of the repository in the Yucca Mountain geological setting relative to the overall system performance standards.

The Total System Performance Assessment supporting the Viability Assessment (TSPA-VA)(CRWMS M&O, 1998d) has now been completed by the Civilian Radioactive Waste Management System Management and Operating contractor (CRWMS M&O) for the U S. Department of Energy (DOE) Yucca Mountain Site Characterization Office and publicly released. Note, however, that the U.S. Environmental Protection Agency (USEPA) has not yet issued proposed standards against which overall system performance will be measured. Regulations have been proposed by the U.S. Nuclear Regulatory Agency (USNRC), but they will be subject to revision once the USEPA standards are set.

The task of the Panel, according to the Peer Review Plan (Appendix B), was to:

> ...conduct a phased review over a two-year period to observe the development and completion of the TSPA-VA. The comments, concerns, conclusions, and recommendations of the final Peer Review Report will be provided to the M&O to support the development and conduct of the License Application TSPA (TSPA-LA). As such, the Panel members will consider not only the analytical approach of the TSPA-VA, but also its traceability and transparency.

The Panel members were to evaluate the analytical approaches used in preparing the TSPA-VA, with specific attention directed to a range of aspects, including:

- physical events and processes considered in the analyses,
- use of appropriate and relevant data,
- assumptions made,
- abstraction of process models into the total system models,
- application of accepted analytical methods, and
- treatment of uncertainties.

These aspects were to be evaluated within the context of their significance to the long-term performance of a repository at Yucca Mountain.

During its two year review, the Panel has discussed and evaluated the adequacy of the total system framework used for the TSPA, the way the individual components of the system were modeled and analyzed, and the significance of the component models to the overall results.

B. Content of Panel Reports

As noted above, the Panel has issued three interim reports, written prior to the completion of the TSPA-VA, and has prepared this final report after reviewing the completed TSPA-VA. A brief review of the coverage in each of the reports is presented below.

Interim Reports

The three interim reports should be viewed as a series. In successive reports, the Panel did not repeat comments found in previous reports except where the Panel amplified, extended, or revised its previous comments.

In its first report (Whipple et al., 1997a), submitted on June 20, 1997, the Panel provided an overview of the TSPA-VA approach and discussed its understanding of processes and events that would affect the long-range performance of a repository at Yucca Mountain and how they were being considered in the TSPA-VA.

The second report (Whipple et al., 1997b), submitted on December 12, 1997, covered general topics that were not covered in depth in the first report and specific issues that the Panel selected because of their potential significance to the results of the TSPA-VA. In addition, the Panel discussed its view of the role of the TSPA-VA, the expectations that could reasonably be set for the TSPA-VA, and how results were being interpreted and limitations and uncertainties were being addressed by the TSPA staff. The report also described in more detail the Panel's understanding of how the processes and events that could affect the performance of a repository at Yucca Mountain were being analyzed in the TSPA-VA.

In the third report (Whipple et al., 1998c) submitted on June 25, 1998, the Panel discussed how the TSPA-VA project staff described the way the repository was expected to work based on what is called the "base case" analysis; the importance to the current analysis of focusing on early canister failures and other events that could lead to releases and doses within 10,000 years; the methodology being used for sensitivity analysis; and, as in the second report, the Panel's understanding of how the processes and events that could affect the performance of a repository at Yucca Mountain were being analyzed in the TSPA-VA.

The Panel provided a summary of its interim findings in each report. The three interim Panel reports are available online at http://www.ymp.gov/reference/va/tspa.htm.

Final Report

As required by the Peer Review Plan, the Panel had two major objectives in preparing this final report:

- To describe the technical strengths and weaknesses of the TSPA-VA.

- To provide suggestions for moving toward the TSPA-LA, if this step is deemed appropriate.

During earlier reviews when complete documentation was not yet available, the Panel supplemented its review of the draft TSPA-VA with formal and informal meetings and interactions with the project staff. In contrast, the Panel's review in this final report is based primarily on documented work, namely, the completed TSPA-VA (CRWMS M&O, 1998d), the supporting Technical Basis Documents (CRWMS M&O, 1998c), and other project documents listed as references to this report.

In Section II, the Panel presents its main findings. These are the issues that the Panel believes are important to the overall credibility and usefulness of the TSPA.

In Section III, the Panel discusses the overall framework of the TSPA-VA, including the uncertainties inherent in modeling the probable behavior of a repository at Yucca Mountain, and draws a distinction between those contributors to uncertainty in performance that can be improved through refinement of models and collection and application of data versus those uncertainties that can be better managed by the use of bounding analyses or design changes. The section concludes with the Panel's recommendations.

In Section IV, the Panel describes its understanding of how the processes and events that could affect the long-range performance of a repository at Yucca Mountain were analyzed in the TSPA-VA and presents its findings and recommendations for each element. As in the interim reports, the discussion follows the major elements examined in the TSPA-VA analysis: (1) initial conditions of the site; (2) conditions as affected by the repository; (3) isolation as provided by the geologic setting in which the proposed repository is to be located, (4) isolation as provided by the waste form and the engineered barrier system; (5) release and transport of radionuclides from the repository; (6) their movement within the biosphere, interaction with exposed population groups, and estimates of the resulting doses; and (7) disruptive events and climate.

II. Main Findings

Although the TSPA-VA is a comprehensive and complex analysis about which few generalizations apply, the Panel has reached a few overall conclusions regarding those issues we consider to be most important to an overall understanding of its strengths and weaknesses. Our findings are often based on or refer to specific aspects of the TSPA-VA, and should be read in the context of the more detailed information provided in Sections III and IV.

A. Reliability of the TSPA-VA Results

Key Points

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.

1. 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.
2. The TSPA-VA was a necessary and useful step in the evolving understanding of how a repository could be expected to perform at Yucca Mountain. It has produced valuable insights into the performance of various repository components, and has helped identify issues where additional data and analyses could lead to improved understanding of the repository's performance. It is also useful in identifying aspects that are comparatively unimportant to performance, for which additional data and analysis are not likely to be beneficial.

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. For example, the comparison of alternative designs based on the estimated doses at a distance of 20 km from the repository and 10,000 or more years into the future requires a degree of resolution that the TSPA-VA may not be able to provide.

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. While it is obviously not feasible to test the full TSPA-VA, it is feasible to test many of the individual component models experimentally. The Panel notes that many experiments are planned or in progress that should be useful in confirming, calibrating, or invalidating the models being applied to analyses of the anticipated conditions at Yucca Mountain. Such experiments cannot be replaced by sensitivity analyses because the sensitivity analyses used in the TSPA-VA often do not directly address the uncertainties associated with the experimental database or the selection of a conceptual model.

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.

Elements of a Credible Analysis

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).
- 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).
- 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.

- 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.

Although the TSPA-VA contains many useful sensitivity analyses that illuminate the system's behavior, these analyses taken as a whole do not provide sufficient insights to overcome the above deficiencies and uncertainties.

In addition to the specific mechanisms that could cause the repository to fail to perform as projected, the overall complexity of the system and the resulting high uncertainties may lead to difficulties in licensing. The USNRC has considerable experience in defining "reasonable assurance" for the licensing of commercial nuclear power plants, but the short time scales and lack of geological complexity of such plants relative to those associated with the proposed repository could be interpreted to mean that the USNRC's experience in defining reasonable assurance may not be applicable to a repository. In the case of the proposed repository, it is possible that "reasonable assurance" will require a degree of proof that is currently not available for the reference design and the site. For example, two aspects of repository performance with large uncertainties are the near-field geochemical environment and actinide transport by colloids. 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.

B. Advances and Improvements in the TSPA-VA Analysis

The TSPA-VA document contains many substantial advances and improvements over the previous TSPA reports issued in 1991, 1993, and 1995. It also provides a revised understanding of how a repository at Yucca Mountain would perform, in comparison to these earlier studies. Perhaps the most dramatic change has been in the estimate of the current infiltration rate, which has been revised upwards by one order of magnitude. This revision has led to many changes in the conceptual models of flow and transport in the mountain, in the repository, and in the saturated zone. In particular, the interpretation by the project staff of flow and transport has shifted from predominantly matrix flow-dominated regimes to fracture flow-dominated regimes that involve fast paths.

A revised scenario on future climates, emphasizing higher rates of rainfall, was also a new addition to the TSPA-VA. The increased rate of infiltration assumed in the analysis leads to the projections of more rapid transport in the unsaturated zone and a larger volume of water coming into contact with waste canisters and waste, a change that, in turn, leads to the projections of earlier and more rapid releases of radionuclides from the waste packages. In response, design changes were made that were intended to strengthen the performance of the engineered barriers. In comparison to previous analyses, the degree to which waste isolation is dependent on the geologic setting has been reduced in the TSPA-VA; the required contribution to isolation from the engineered barriers has significantly increased.

The revised interpretation of infiltration has led to a more realistic, although still far from complete, representation of the fracture-matrix interaction and to an improved characterization of the hydrologic properties of the mountain. Although much is still unknown and/or uncertain, there have been several advances in addressing the problem of modeling the performance of the site. A significant development in the current TSPA-VA is the incorporation, for the first time, of a model of seepage into the drift. This addition relates to the hydrology of the near-field environment, which is modeled at a scale much smaller than in the previous TSPA reports. Drift-scale hydrology critically affects the rates of canister failure, and thus represents a key consideration in the analysis of repository performance. The , currently under way, and other investigations in the engineered barrier system will be useful in testing the current models. The hydrology at this scale is also linked to processes at the mountain scale, at least during the thermal period, and to thermal-hydrologic, thermochemical, and thermomechanical processes. The coupling of these processes was not considered in the TSPA-VA.

Substantial improvements have been made in the modeling of flow and transport at the various space and time scales, and in the linkage between these scales. The Panel notes, in particular, advances in the use of more sophisticated numerical models such as the dual permeability model, the finite element heat and mass model, and particle-tracking, and decreasing reliance on the limited equivalent-continuum model. The hybrid approach for assessing the effects of thermohydrologic processes at different scales and from different heat sources, in a computationally manageable scheme, as illustrated in Chapter 3 of the Technical Basis Document (CRWMS M&O, 1998c), represents a significant improvement, even though it is far from complete.

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.

The project team and its supporting contractors have made advances that have not been included in the current version of the TSPA-VA. Many of these are improvements in basic scientific issues, and they lead to an improved understanding of fundamental processes and the projected repository performance. Of particular significance are the analyses of coupled thermohydrological, thermochemical, and thermomechanical effects described in publications by Wilder (1996), Hardin and Chesnut (1997), and Hardin (1998). These represent serious attempts to study the complex interaction problems resulting from the thermal pulse. Also worthy of note are the sensitivity analysis of saturated zone (Arnold and Kuzio, 1998), the introduction of geostatistics for assessing flow, transport and retardation in the unsaturated zone; and the analyses of the various tests currently under way, including the single heater test, the large block test, and the .

C. Key Role of the Waste Package

Corrosion Resistance

Based on the TSPA-VA results, the analysts have judged that the rate of waste package degradation is a principal determinant of overall repository performance. Hence the integrity of the waste package as a barrier is crucial to the performances of the repository as projected within the TSPA-VA for each of the time periods considered: 10,000, 100,000 and 1,000,000 years (CRWMS M&O, 1998d, pages 0-16). The Panel agrees that this is a logical and credible conclusion. Therefore, it is important that the factors that control the life of the waste packages be carefully identified and analyzed.

Corrosion is the most important and realistic threat to the deterioration of the waste packages. Although an outer canister of steel will readily corrode in hot, moist conditions, under the proper environmental conditions (temperature-relative humidity-water chemistry), C-22, a proposed waste canister material, can realistically be expected to remain passive for long periods of time. Since such conditions are anticipated to prevail within the proposed repository, it is likewise anticipated that C-22 will corrode at an extremely slow rate. At this stage of development, however, the analyses leading to this assumption are necessarily a simplification of a complex problem and far from rigorous.

Need for Data

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.

In the case of the TSPA-VA, estimates for both of these factors were based on expert elicitation. Although a large number of models that are reasonable and well conceived have been developed for evaluating various waste package processes, few of these have been validated and/or verified through the use of experimental data. In fact, experimental data are lacking throughout the treatment of the waste package and engineered barrier system (WP/EBS). These deficiencies will need to be resolved prior to the preparation of the TSPA-LA.

Wet Waste Packages

Because the spatial and temporal pattern of water seepage onto the waste packages is highly uncertain, it is prudent to design them with the anticipation that they will be wet during significant periods of time. The extent that waste packages are not wetted or are wetted to a lesser degree can be accepted as a source for increased confidence in the barrier properties and a hedge against uncertainty.

The waste package surface will be dry when it is above a critical temperature (T_{WET}) for the formation of a moisture film. This condition is expected to pertain after emplacement. It will persist until the waste packages cool below the temperature where moisture is stable. In the TSPA-VA, estimates for the critical temperature for moisture formation are based upon expert elicitation. Increased concentrations 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. With respect to corrosion, the important properties of the moisture that forms on the waste package surfaces are chemical composition, the level of acidity (pH) and the oxidizing power (Eh). In the TSPA-VA, all of these important properties were based upon expert elicitation. Experimental data are required in this important area.

When the waste package surface is wet, the important issue becomes whether the metal has sufficient corrosion resistance to remain passive (and therefore to corrode at extremely slow rates), or whether localized corrosion will occur. In the TSPA-VA, the treatment is based on the concept of a critical temperature (T_{CRIT}) for localized corrosion. At temperatures in excess of this, localized corrosion can persist. Conversely, at lower temperatures, localized corrosion will not persist and the metal will remain passive. The difference between these two temperature limits (T_{WET} and T_{CRIT}) determines the critical temperature range in which localized corrosion can occur, i.e., at temperatures low enough for moisture to form and yet high enough for localized corrosion to occur. The time-temperature profile of a waste package will determine the time at which the critical temperature range is entered and the time duration that the package remains within this range. If the critical temperature for the metal is higher than the temperature for moisture formation, then no localized corrosion is expected to occur.

The Panel concludes that this approach to localized corrosion is sound and consistent with the current knowledge of corrosion science and technology. 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.

Use of the TSPA to Evaluate Design Options

Although the project staff has adequately and convincingly determined that waste package performance is critical, the TSPA is only one of several methods for the evaluation of base case design features and for the comparison of the base case with alternate designs. 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.

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. These efforts should focus on the processes and components at the micro-level; they should not be aimed at the macro-level of the overall repository. The devil is in the details, and the details are lost at the overall repository response level. For example, the performance of the waste packages depends on the specifics of the methods used in their manufacture and fabrication. Alternative welding procedures are not amenable to evaluation within the TSPA; rather they need to be evaluated in the supporting documentation and engineering analyses. Development of an improved information base at the process level will increase the confidence in the TSPA results.

D. Key Role of Infiltration and Seeps Analysis

According to the TSPA-VA report, "limited water contact of waste packages" is one of the four basic attributes of the proposed repository. Infiltration and seepage into drifts are the main factors which control water contact with the canisters.

The base case in the TSPA-VA assumed that seepage into drifts is negligible during the thermal period, which was predicted to last for a few thousand years. Following the thermal period, seepage rates into the drifts were calculated by assuming a steady-state, in which the percolation rate near the drift was equated to the infiltration rate beneath the land surface, directly above the particular drift. The infiltration rate was estimated from the infiltration maps and the assumed climate. It was further assumed that the thermal period has no significant effect on the drift-scale hydrologic properties, which were taken in the analysis to be the same as present-day properties. The fraction of canisters that get wet and the corresponding seepage rates were determined from a random sampling of a response surface obtained from a detailed analysis of seepage in an individual drift. This probabilistic approach reflects the uncertainty in the capillary and flow properties of the fractures at the drift-scale.

In the base case, the project staff conservatively ignored the effect of the matrix, which would be to delay the onset of seepage and to reduce the seepage rates. The assumption in the seeps analysis that all percolation flows through fractures led to a conservative estimate of seepage. The analysis predicted a percolation flux threshold (in the range of 2-3 mm/yr) such that for percolation rates below this threshold, seepage does not occur. Above this threshold, the seepage rate was found to be a non-linear increasing function of the percolation rate. However, the results depend sensitively on the permeability and capillary structure of the fracture continuum in the immediate neighborhood of the drifts. As a result, the base case projections are subject to the large uncertainties in the knowledge of the heterogeneity, spatial correlation and anisotropy of these properties.

Figure 3-13 of the TSPA-VA, for example, shows that for a wide range of percolation flux values, the variance in the seepage fraction is almost equal to its mean value. It is not surprising therefore, that seepage into drifts was found to be one of the most sensitive parameters in the final dose results in the TSPA-VA report.

Of interest is the predicted sensitivity of the seepage fraction on the percolation flux for values above the threshold and below 10 mm/yr, as shown in Figure 4-3 in Volume 3 of the TSPA-VA (CRWMS M&O, 1998d). On the basis of data presented in this figure, it follows that predictions of the fraction of wet canisters under present-day infiltration, which falls in this range, will be subject to relatively large uncertainties. This underscores the need for an accurate estimate of the magnitude of the percolation flux. In the long term, the effect of percolation rate, *per se*, on seepage cannot be estimated with a large degree of accuracy, given the uncertainties in long-term climate predictions.

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 rockfalls. Damage to the drifts would alter seepage rates and locations in two ways: As a result of the different boundary condition at the drift ceiling and as a result of the presence of rockfall on the canisters. These two combined effects will alter the predictions on seepage patterns and rates and the contact of waste packages with water.

The hypothesis that negligible seepage occurs during the thermal period is based on certain assumptions of spatial homogeneity and symmetry. However, the possibility cannot be excluded that episodic seepage events will occur during the thermal period, in which canisters get wet as a result of instabilities at the overlying heat pipes or of focused flow, driven by heterogeneities in flow properties, canister heat output, and canister location (edge vs. center). Episodic seepage during the heating period was recently observed in the large block test (Hardin, 1998). If this were to occur in the proposed repository, it would lead to premature canister wetting in some locations. The absence of such a possibility needs to be convincingly and unambiguously demonstrated.

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.

Finally, the Panel notes that waste packages at the edges of, or in isolated zones within, the repository may differ considerably from the standpoint of their exposure to water. Another uncertainty, in addition to the volume and distribution of water flowing, is whether water flows as droplets, films, or streams. The effects of rock particulate, debris, backfill, and corrosion products on water distribution and time-of-wetness were not well defined in the TSPA-VA.

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.

E. Potentially Non-Conservative Aspects of the Analysis

Cladding

The outcome of the TSPA-VA analysis depends to a considerable extent on the performance of the fuel cladding (CRWMS M&O, 1998c, Chapter 4, see page 4-12 and Figure 3-54), 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 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. The TSPA-VA (page 3-101) cited the work of Rothman (1984) in the discussion of oxidation rates for Zircaloy as part of the basis for the credit taken for extended cladding lifetime. This same paper notes,

    > Finally, insufficient information is currently available on stress-corrosion cracking. While evidence is presented that SCC failure is not likely to occur, it is difficult to demonstrate this conclusively because the process is not clearly understood and data are limited. (page ii)

2. As noted in the TSPA-VA (page 3-102), Zircaloy may be susceptible to corrosion under certain chemical conditions. The authors of the TSPA-VA noted, "However, the chemistry within the waste package, hence the long term performance of Zircaloy cladding, is not well understood and has considerable uncertainty." Additionally, stress corrosion cracking is sensitive to chemical conditions (see extensive literature survey in Sidky, 1998). These chemical processes were explicitly not considered in the TSPA-VA (Siegmann, et al., 1996, page 16).

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.

4. Although the Panel strongly urges that the project team initiate and complete the necessary experimental programs, we note that time is limited. Quoting from Siegmann et al. (1996):

> Development of testing data for such purposes is both lengthy and costly, and may not be practical in view of the time limitations for the licensing. The most practical approach for an immediate use would utilize the data available in the literature. (page 16)

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" (TSPA-VA, page 5-25). 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.

Soil Buildup in Biosphere Analysis

As part of its biosphere analysis, the project staff has estimated the doses that would result from the use of contaminated groundwater for drinking and irrigation. Inhalation of dust containing radionuclides that would be found in irrigated soils has also been evaluated. Such an analysis has many components, including the estimation of the quantity and type of foods consumed, the factors that indicate how radionuclides in water are transferred to soil, from soil to plants, and, for forage crops, from plants to animals.

The quantities of radionuclides that are assumed to transfer from soil to plant roots depend on their concentrations in the soil, and these concentrations can increase with ongoing irrigation with contaminated water. Eventually, a steady-state condition is reached in which the annual radionuclide additions to the soil through irrigation with groundwater will be equal to the annual losses. Soil losses can occur by wind or water erosion, and radionuclides can be removed from surface soils by transferring to crops that are subsequently harvested, or by weathering into the soil below the crop root zone.

The analyses of the biosphere dose conversion factors were conducted using the GENII-S model (Leigh, 1993). This model permits the user to specify the length of time that irrigation water is deposited on the soil prior to the intake period for which a dose is estimated. In the 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 soil near release sites for iodine (Kantelo et al, 1982, Straume et al., 1996, and Straume et al., 1997). 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 by which the dose is underestimated could be significant.

F. Potentially Conservative Aspects of the Analysis

Transport through Penetrations in Waste Packages

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. This is due in part to the preliminary state of the analysis of the likely evolution of penetrations through a damaged waste package. 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, the distribution of penetrations on an individual waste package, 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. The results of these efforts will be coupled to and have a significant effect on several other process models and abstracted models. The important parameters are (1) the time sequence of waste form exposure to the repository environment; (2) the transport of water and other species into the waste packages; and (3) the release and transport of radionuclides from the waste packages.

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. Waste package penetrations from general corrosion are likely to be broad patches ranging from a few centimeters to tens of centimeters in diameter. The spatial distribution of penetrations at the top or bottom and along the sides of the waste packages is poorly understood and defined. The issue of the likelihood of penetrations remaining open or becoming blocked by corrosion products or deposits, has been introduced, but the understanding is not well developed. Once a waste package has been penetrated, water and air from outside will have access to the waste package internals and the spent fuel. The subsequent processes that ensue among internal metal structures, cladding, and spent fuel were not addressed in any depth within the TSPA-VA.

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.

Retention of Radionuclides in Alteration Products of Spent Fuel

As discussed in the first interim report of the Panel (Whipple et al., 1997), the alteration and corrosion rate of UO_2 is relatively rapid under moist, oxidizing conditions. As modeled by the TSPA-VA (CRWMS M&O, 1998C, Chapter 6, Section 4.6.2.2.2), the UO_2 in the spent fuel will be completely converted to secondary uranyl phases within 100 to 1,000 years after waste package and fuel cladding failure and exposure to water. In the present analysis, the corrosion of UO_2 results in releases of radionuclides which are then available for transport in water, and only the solubility limits for individual radionuclides place an upper limit on the radionuclide concentrations in water. However, under such conditions, an assemblage of secondary uranyl oxyhydroxides, silicates, and carbonates will form depending on groundwater compositions. It is expected (Burns et al., 1997) and has been shown experimentally (Buck et al., 1998) that certain radionuclides, such as ^{237}Np, will be incorporated into the structures of these secondary phases. Thus, the formation of these secondary alteration phases may remove certain radionuclides from solution by co-precipitation or sorption and retard their release from the near-field environment.

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.

Potential Sorption of Technetium and Iodine

The TSPA-VA analysis of the performance during the first 10,000 years after repository closure indicates that the calculated doses are due to ^{99}Tc and ^{129}I. Ultimately, the doses from neptunium and plutonium are estimated to be larger, but these radionuclides are not expected to reach the accessible environment in significant concentrations until much later, because their flow through the unsaturated and saturated zones is assumed to be retarded by chemical sorption. No retardation credit is taken for technetium and iodine (or for three other radionuclides), based on the lack of observed sorption in batch measurements of K_d values. The decision is described in the TSPA-VA as conservative.

However, the data cited above regarding the potential accumulation of iodine in surface soils (Kantelo et al., 1982, Straume et al., 1996, Straume et al., 1997) indicate that iodine deposited on the ground from the Chernobyl accident is retarded in the upper soil layer to about the same extent as is plutonium and cesium. Given these data indicating that iodine does not move readily through soil, it could also be the case that iodine could be retarded in transport through the unsaturated and saturated zones. The Panel has not conducted a literature review on this issue.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 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 reprocessing. Although it appears that some fraction of the deposited radionuclides may be transported to groundwater, as was the case with cesium at the Hanford tank farm, field data suggest that radioiodine does not move unretarded through soil.

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.

G. Potentially Important but Omitted Processes

The Panel has identified several processes that can have major detrimental effects on repository performance, but which are currently not extensively analyzed. These processes require further analysis and an assessment of their importance.

Expansion of Steel Corrosion Products

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. When steel corrodes, the iron oxide that forms occupies a volume two to three times larger than the corroded metal. When these corrosion products form in tight spaces, e.g. the crevice between the outer steel barrier and the inner C-22 barrier of the base case design, high stresses are produced that will lead to plastic deformation of the remaining metal structures. Such "pack-out" failures have been observed for structural steel beams where atmospheric corrosion caused the expansion of steel corrosion products. "Denting" failures of nickel alloy tubes in steam generators in nuclear power plants were caused by iron oxide growth due to corrosion of the steel support plates. This process represents a serious threat to the integrity of the inner C-22 barrier of the waste package, once the outer steel barrier has been penetrated and water gains access to the crevices between the barriers.

Hydrogen Embrittlement of Zirconium Cladding

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.

Stress Corrosion Cracking

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.

H. Data Needs

The Panel is 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.

Fundamental Data

A substantial part of the knowledge base, presently rests on expert elicitations (Table 3-2, page 3-2 of the TSPA-VA) 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.

Solubility limit distributions for the key radionuclides (Table 3-15, page 3-99 of the TSPA-VA) have only a limited experimental basis. Indeed, most are based on expert elicitations or a reanalysis of previous experiments. If there is any area amenable to experimental study, it should be the determination of concentration limits in relevant solution compositions. Project scientists are well aware of the need for data, particularly for actinides (Near-Field/Altered-Zone Models Report, page 5-15). The NEA data base for uranium (Grenthe et al., 1992) has thermodynamic data for fewer than five uranyl oxyhydroxides and silicates that may be important during the corrosion of the UO_2 in spent fuel. In 1993, J. Fuger reviewed the database for actinides, and concluded that not only are there inconsistencies in the database for uranium, but that for the transuranium elements many fundamental data are lacking. The present situation is not much improved.

An experimental program should be developed to advance the spent fuel corrosion model beyond its present empirical representation by a response surface. "Currently, detailed knowledge is not available for the atomic (mechanistic) steps and the sequence of chemical/electrochemical reaction steps to describe the dissolution process over the range of spent fuel inventory, potential water chemistries, and temperatures" (CRWMS M&O, 1998c, Chapter 6, page 6-60). Since over ninety percent of the radioactive waste intended to be disposed in the repository is spent fuel, a considerable knowledge of spent fuel corrosion is likely to be required.

There are similar lacks of data for Zircaloy cladding corrosion, secondary phase formation, colloid formation and transport, K_d, and saturated zone characterisitics.

Testing Models

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 data base or the selection of a conceptual model.

Concerning field tests, many of the questions raised about the effects of the thermal pulse can be (at least partly) answered from the results of the , which is one part of the in situ thermal testing program (DOE, 1995) for Yucca Mountain. This test is an important experiment that will provide the first large scale underground investigation of the thermomechanical and thermochemical processes which control the thermal behavior of the rock mass surrounding the proposed repository. The Panel believes that the 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. Underground testing in fractured tuff on this scale has never before been performed. It is anticipated that the results will provide data that will lead to a reduction of uncertainties.

I. Insights from the TSPA-VA

The Panel observes that the analysis indicates that the performance of the proposed repository depends primarily on the functions and efficiencies of certain major elements of the system. The TSPA-VA (Section 2.2.1) describes the four key attributes that contribute to the safety of the repository as:

- Limited water contacting waste packages;
- Long waste package lifetime;
- Slow release of radionuclides from waste package; and
- Reduction in the concentration of radionuclides during transport from the waste package.

These four attributes of the repository system control the radionuclide concentrations that may ultimately reach the accessible environment. These system elements, in turn, can be grouped into two spatial and functional groups:

- Near-field: delay in the release and mobilization of radionuclides; and
- Far-field: transport of radionuclides, with associated delay and dilution.

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.

From the perspective of the time frames associated with peak doses, it is the case that the major share of protection comes from the engineered barriers, along with whatever dilution occurs in the saturated zone. But for an initial 10,000 year assessment, the relative contributions from the initial thermal period and from the travel times through natural barriers are more significant, in a relative sense, in delaying the arrival of radionuclides at the accessible environment. The thermal period is projected to prevent the onset of liquid water reaching the waste packages for around 2,000 years, and the travel times for transport in the unsaturated zone and saturated zone are estimated to be around 1,000 years for nonretarding radionuclides, and longer for the others.

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. These four attributes can be presented in a framework that includes the supporting models and their underlying physical and chemical principles, conformance with available laboratory and field data, experiences with similar models in comparable systems, and sensitivity analyses based on alternative plausible models. If such a framework can be effectively developed, the strategy of "defense-in-depth" will have been applied successfully to the design and analysis of the proposed repository.

III. THE TSPA-VA METHODOLOGY

In this section, the Panel discusses the overall framework of the TSPA-VA, including the uncertainties inherent in modeling the probable behavior of a repository at Yucca Mountain. A distinction is drawn between those contributors to uncertainty in performance that can be improved through the refinement of models and the collection and application of data, versus those uncertainties that can be more effectively managed through the use of bounding analyses or design changes. The section concludes with the Panel's recommendations.

A. Expectations for the TSPA-VA

Differing Objectives for the TSPA-VA and the TSPA-LA

As part of its review, the Panel considered the relation between the TSPA-VA and the TSPA-LA. The Panel's Peer Review Plan addresses this issue: "The Peer Review Panel members will conduct a phased review ... to observe the development and completion of the TSPA-VA. The comments, concerns, conclusions, and recommendations of the final Peer Review Report will be provided to the M&O to support the development and conduct of the License Application TSPA (TSPA-LA)."

The Congressional mandate that a viability assessment be conducted was stipulated in the Energy and Water Development Appropriations Act of 1997. Specifically, the Congress directed DOE, in the course of this assessment, to analyze "the probable behavior of the reference design for the engineered repository components in the expected natural conditions at the Yucca Mountain site." If the project moves on to the license application phase, the goal will be different. The USNRC, for example, in 10 CFR Part 60 and in its draft regulations in 10 CFR Part 63 for the proposed Yucca Mountain facility, has stipulated that the goal is to provide "reasonable assurance" that a facility of this type will comply with its regulations. While it is not possible for the Panel to know at this time how this requirement will be interpreted, it is our opinion that the Commission may likely require a higher standard of proof than is associated with the Congressional concept of "probable behavior" at the VA stage. That is to say, the USNRC may require that the results be developed and defended in a manner so as to demonstrate a higher level of confidence. At the same time, however, it is important to keep in mind that neither the USEPA nor the USNRC expects DOE to be able to perform an assessment that provides proof positive that the proposed repository will perform in a given manner.

In addition to the degree to which the TSPA-VA and TSPA-LA may require different goals for the analyses, the Panel noted in its third report that the draft TSPA-VA analysis was based on models that may be better suited for estimating peak doses at some later time than for assessing performance within the first 10,000 years. At the LA stage it will be necessary to estimate the performance during the time frame specified by the regulations. Based on draft guidance from the USNRC and on recommendations to the M&O from the DOE, it is anticipated that this time frame may be 10,000 years. Given these fundamental differences in the objectives for the degrees of certainty and the time frames of the TSPA-VA and the TSPA-LA, it follows that the two analyses may differ significantly.

In addition to meeting the needs of the VA and LA, a version of the analysis will be required in support of the preparation of the associated Environmental Impact Statement (EIS). Performance assessments will also be necessary for evaluating various alternative designs. The degree to which the EIS and the design review analyses will address "probable behavior," versus a determination of "reasonable assurance" of performance, is a consideration for the TSPA staff. It is beyond the scope of this peer review.

The main point of the Panel in noting the differing objectives for the TSPA-VA and the LA is to make it clear that there are several options available to the TSPA staff to address deficiencies in the VA. Certain of these deficiencies are noted in Section IV of this report. Several approaches that the TSPA staff may want to consider as the analysis moves forward to the possible LA phase are addressed in Section III.D.

Inherent Uncertainties in the Assessment

In developing its standards for the geologic disposal of radioactive wastes, the USEPA recognized that large uncertainties would be associated with performance assessments over long time scales. For this reason, in 40 CFR Part 191.13(b) of its standards for spent nuclear fuel and high-level and transuranic radioactive wastes (which now apply to the Waste Isolation Pilot Plant, but not to the proposed repository at Yucca Mountain), the Agency included the following statement regarding the degree of confidence that one must have that the containment requirements are met:

> Performance assessments need not provide complete assurance that the requirements of Sec. 191.13(a) will be met. Because of the long time period involved and the nature of the events and processes of interest, there will inevitably be substantial uncertainties in projecting disposal system performance. Proof of the future performance of a disposal system is not to be had in the ordinary sense of the word in situations that deal with much shorter time frames. Instead, what is required is a reasonable expectation, on the basis of the record before the implementing agency, that compliance with Sec. 191.13 (a) will be achieved.

As the USEPA noted, factors such as the complexity of the total system, the variability in the natural setting, and the need to estimate the performance of the repository over extended periods of time result in large inherent uncertainties. These uncertainties, in turn, have an impact on the overall credibility of the TSPA-VA. Many uncertainties are evident in the characterization of the site, in the development of conceptual models, in the selection of values for various input parameters, and in the determination of boundary conditions. Other uncertainties developed as an outgrowth of the presence of the novel and not yet field-tested aspects of the analyses of the many processes that may occur in a geological setting. The TSPA-VA staff acknowledged these uncertainties and devoted a large fraction of their report to a discussion of the associated probability density functions and sensitivity analyses.

For these and other reasons, it is important that the TSPA staff continue to recognize the limitations that these uncertainties place on their analyses, especially as they move into the LA phase. The Panel has been mindful of the need to acknowledge, in the course of our review, what is feasible and what is not.

B. Methodology

Overall Framework of the Analysis

The Panel concluded that the overall performance assessment framework and approaches used in the TSPA-VA are sound and follow accepted methods for risk analysis. However, some of the technical complexities associated with the analysis are unusual if not unique.

Conventional Aspects

The project staff has followed conventional methods in the TSPA-VA analysis in that it:

1. Begins with the characterization of the inventory of radioactive materials to be placed in the repository.
2. Characterizes the site.
3. Conducts analyses of the processes and events that could cause the engineered barriers to fail and radionuclides to be released. Such barriers include the waste form, the cladding, and the waste package. The outcomes of these analyses provide estimates of the rate of release of radionuclides through each of these barriers and form the basis for subsequent calculations of radionuclide transport and exposures.
4. Accounts for radioactive decay, both during the time prior to the release of radionuclides from the waste packages and during their transport through the environment.
5. Models the transport of the released radionuclides through the unsaturated zone, with consideration given to mechanisms that would lead to retardation of certain radionuclides.
6. Models the transport of the radioactive material within the saturated zone. This analysis includes retardation and dilution, and leads to a projection of the concentration of key radionuclides in groundwater at offsite locations where people could be exposed.
7. Considers a full range of pathways in the exposure assessment, including the direct consumption of groundwater, ingestion of foods contaminated through the use of groundwater for irrigation, inhalation of contaminated dust, and direct radiation from the ground surface.
8. Evaluates several exposure scenarios, in which the principal differences are with the assumed fractions of locally produced foods consumed by members of the exposed group.

Novel Features

The TSPA-VA includes several features and analyses that are novel. These include the:

1. Unprecedented time periods over which the analyses were performed. The TSPA-VA extends from up to 10,000 to up to 1,000,000 years into the future, with unknown changes occurring over those times (e.g., climate, locations of people and their sources of food and water). These time periods are also long compared to those

available for testing the corrosion rates of materials, thus making the extrapolation of materials performance uncertain.

2. Length (20 kilometers) of the subsurface pathway over which transport was modeled.
3. Heterogeneity of the site and of the paths through which radionuclides could be transported and ultimately come into contact with people. The movement of radionuclides occurs as a result both of water flow through fractures and its interactions with the rock matrix. The site cannot be characterized at a sufficiently detailed scale to define precisely the flow paths or material interactions.
4. Complexity of the processes that interact to affect hydrologic and chemical conditions within the proposed repository and adjoining areas. The coupled interactions among heat, moisture, and the chemical environment, and the responses of the proposed repository to the associated mechanical stresses are complicated and cannot be modeled with precision. Material performance will depend on the thermal, chemical, and hydrological environments as they evolve over time, yet material performance can also alter these conditions, e.g., corrosion byproducts from steel may affect water flow, colloid formation, and water chemistry. The site conditions measured during the site characterization phase of the project may be significantly altered by the heat output of the waste.
5. Sensitivity of the performance of the proposed repository to features that cannot be precisely assessed. For example, if the infiltration rate of water through the mountain is higher than anticipated (or if climate changes lead to wetter conditions), there will be an increase in the portion of unsaturated zone flow through fast pathways, in the number of waste packages in contact with seeps, and in the amount of water contacting waste packages. Such enhanced flow will result in increased releases of solubility-limited radionuclides. At the same time, the lifetimes for the waste packages and the time required for radionuclides released from the waste packages to reach the saturated zone would both decrease.

These novel features limit the confidence that can be placed in the outputs of the TSPA-VA.

Use of Model Abstractions

Because of the inherent complexity of the proposed facility and site and the number of simulations that need to be analyzed, the detailed process-level models are abstracted, i.e., replaced with simplified models or with lookup tables generated by the underlying process models. The purpose of this approach is to reduce the computational requirements associated with the analyses. The Panel agrees that this approach is sound in principle. For example, the use of model abstractions avoids the need to conduct numerous runs of the complex biosphere analyses, incorporating a host of individual assumptions regarding the multiple possible exposure pathways and food consumption rates for each model realization. Instead, the results of a series of biosphere analyses can be used to generate distributions for the doses that would result from a specified groundwater concentration of each radionuclide under consideration. These distributions, referred to as biosphere dose conversion factors, are used in the integrated TSPA calculations to estimate doses. This approach is computationally efficient and technically appropriate. In addition, the use of abstractions may prove helpful in future licensing reviews by making it easier to separate the evaluation of the component models from the consideration of how the results of these models are integrated into the overall analysis.

For several of the mel 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" (CRWMS M&O, 1998c, Chapter 4, page 4-38). 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.

Uncertainty and Sensitivity Analyses

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. Even with these limitations, however, the sensitivity analyses can be valuable if it can be shown that certain aspects of the repository system have little effect on the performance of the repository. However, 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.

In seeking to understand the performance of the proposed repository, the TSPA-VA staff has, in general, modeled the various issues separately. In some cases, they have performed limited coupled-process analyses. They have also conducted a variety of sensitivity studies and bounding-type evaluations, typically to examine how the estimated overall performance of the proposed repository depends on a single parameter or aspect, while holding constant the other interacting parameters or aspects. One example was the evaluation of thermomechanical effects in the unsaturated zone, which were not incorporated in the base case analysis.

While it may be possible to analyze some components and systems in a realistic manner, the analysis of others may of necessity, because of data or modeling limitations, have to be based on bounding and therefore conservative assumptions.

This can lead to several problems:

1. Sensitivity analyses may indicate incorrectly that a particular feature of the site or design is unimportant to performance. This could be the case, for example, where the given feature has been analyzed by an overly conservative bounding analysis. When a parameter point value is used, a sensitivity analysis typically cannot identify whether that parameter is important or unimportant to performance.
2. Similarly, a sensitivity analysis may be performed over too narrow a range of values to reflect the actual sensitivities. It is important that a full range and distribution of the uncertainties in the values for each key input parameter be considered, and appropriately justified. An analysis that may be unrealistically optimistic can mask the actual sensitivities in the performance of that system and/or component. For example, the cladding analysis produces an estimate of the cumulative cladding failures over time. The lower bound of the failure rate curve (that is, the "worst case") indicates that the cladding is so robust that repository performance is comparatively insensitive to this aspect of performance.
3. It may be difficult to assess the relative importance of components and systems.

In its first interim report, the Panel discussed the importance of viewing sensitivity analyses from multiple perspectives and over differing periods of time. At that time, the Panel noted that, while an aspect of performance may not seem important when viewed from an overall perspective, it may be important on the basis of considerations of subsystem performance measures. The TSPA team has been responsive to this recommendation. 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.

Use of Expert Elicitations

Several of the more important components of the TSPA-VA were based on information derived through expert elicitations. The results of these elicitations have been used in analyses of the probabilistic volcanic hazard, probabilistic seismic hazard analysis, waste-package degradation, and radionuclide mobilization, saturated-zone-flow issues, radionuclide solubility limits, and near field/altered zone coupled effects. The expert elicitations followed a defined protocol and were extensively documented.

The value of a properly executed expert elicitation under these circumstances is that it provided the TSPA-VA staff with the full, and fully documented, range of interpretations of the data or models currently considered valid or respectable. Such a process can also, if properly applied, direct the thinking of the experts toward the specific questions being faced, including where the data or models need to be applied and how. Through the process of being forced to interact on the subjects at hand, the experts can often resolve conflicting interpretations and provide a more unified view than the TSPA-VA staff could reach on its own.

Nonetheless, 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. However, there were several positive results from the use of expert panels that clearly make evident their value to the project. One major contribution, in a general sense, was in challenging the TSPA-VA staff's basic approach to, and conceptual modeling of, a particular issue. For example, the streamtube analysis used to assess the transport of radionuclides in the saturated zone was developed in response to criticisms of the previous model by the expert panel. A second benefit was that often the experts were able to identify relevant studies or data with which the TSPA-VA staff members were not familiar.

On balance, the contributions from the expert panels to the TSPA-VA were positive. The panels improved the analysis of many component parts of the TSPA-VA. Although there are some issues for which expert opinion (rather than laboratory data) served as the primary basis for estimating the projected performance of the proposed repository, the process through which the experts worked generally provided adequate feedback to enable them to confirm whether their opinions were appropriately used in the assessment. This process should not be seen by the project staff as completed; expert opinions should not be used when the required data can be obtained from experiments or field studies, in a reasonable amount of time.

Use of Expected Values

The results of the TSPA-VA analysis are presented in terms of the expected values of the doses, calculated as a function of time, based on multiple runs (or realizations) of the system of models. In these model runs, the ranges of parameter values were sampled according to their estimated underlying probability distributions. These calculations are probabilistic in the sense that each run involved estimation of the fraction of waste packages that experience seeps; the fraction that have failed through corrosion at any given time was estimated probabilistically. In addition to the expected value, curves reflecting the fifth and ninety-fifth percentile distributions were provided in some cases. This approach follows the normal and accepted methodology for such analyses.

However, the results need to be understood in the sense that the expected (or mean) value of a calculation is not necessarily informative about the nature of the underlying distribution. For example, a scenario that leads to a dose rate of 1 mrem per year has the same mean value as an event with a 1% probability per year of occurring, and which results in a dose rate of 100 mrem per year if the event occurs. In this latter case, the expected value for the scenario is 1 mrem per year, but 1 mrem per year need not be a likely or even possible result of the event. While these two cases have equal expected values, they may not be viewed as equivalent risks.

The situation where the expected annual dose does not describe the results of specific scenarios occurs in the TSPA-VA at "early" time periods. At early times, a single juvenile waste package is assumed to occur at 1,000 years, presumably due to poor fabrication. Isolated waste package failures are also estimated to occur due to corrosion within the time period between several thousand years to ten thousand years after repository closure. As described in Section IV, the analysis assumes that stainless steel cladding (slightly over 1% of the total spent fuel) provides no barrier to the release of radionuclides. In addition, a smaller amount of spent fuel is assumed to have cladding that is not completely intact at the time of disposal. In total, 1.25% of the spent fuel is assumed to lack a cladding barrier when the waste package fails.

It is unlikely that the stainless steel clad fuel will be uniformly distributed throughout the waste packages. For this reason, the juvenile failure of one waste package will most likely involve no immediate release of radionuclides, assuming that the cladding is intact and acts as an effective barrier. But for 1.25% of the time, the full contents of the waste package are available for release and transport after waste-package failure. The analysis treats the source term for the juvenile failure as equal to 1.25% of the inventory of the average package of spent fuel, and the annual dose due to a juvenile failure is calculated on this basis. It may not be clear to the TSPA-VA reader that the estimated annual dose is an expected value resulting from 98.75% of scenarios that produce no radiation exposure and 1.25% that produce exposures that are higher than the mean (higher by a factor of 80, in this example).

C. Complexities of the System and of Its Components

Modeling of Coupled Processes

One critical aspect of the TSPA-VA is the degree to which an appropriate conceptual model and approach were applied to three key groups of phenomena that involve complex coupled processes or data-intensive analyses of a large heterogeneous site, as exemplified by Yucca Mountain. These are:

- Phenomena in the unsaturated zone above and near the repository during the first several thousand years that govern whether the various waste packages will be wetted, will be in a humid environment, or will remain essentially dry;

- Waste-degradation phenomena inside the waste packages, after canister degradation has begun, that govern how much, how quickly, and in what forms the radionuclides may move from outside the waste packages into the local environment; and
- The behavior of the radionuclides in the unsaturated and saturated zone environments.

It is difficult to model adequately each of these sets of phenomena over the anticipated 10,000-year regulatory period. For the first two groups, this difficulty is due to the fact that each is influenced by complex coupled interactions. Phenomena in the unsaturated zone involve a combination of thermal, hydrological, mechanical, and chemical processes and effects; in the waste-degradation process, they involve a combination of physical, chemical, and mechanical processes and effects. For the third group of phenomena, the difficulty stems from the heterogeneity of the site and the large distances over which the transport of radionuclides is to be assessed. It is not feasible to know the structure of the flow paths in sufficient depth to model these phenomena in detail.

In neither of the first two cases were sufficiently detailed coupled models developed in the TSPA-VA to permit an integrated analysis to be performed. The development of a fully-coupled model based on first principles for the reference design may be beyond current analytical capabilities. Making such an analysis especially difficult is the lack of an adequate theoretical basis for such models, compounded by the lack of sufficient site-specific data to support them.

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. The ongoing thermal testing program is designed to investigate precisely these issues, namely, to provide data that will lead to a better definition of the effects of coupled processes. The Panel addresses these issues in Section IV.

Limitations of the Component Models

The Panel's detailed comments on the TSPA-VA component models are presented in Section IV. Although many of the processes addressed in the TSPA-VA are extremely difficult to analyze and would perhaps be better addressed through bounding analyses, the Panel has reviewed the application and analyses produced by these component models against the Congressional charge to assess the probable behavior of the repository system. As discussed in the Panel's Second Interim Report (Whipple et al., 1997), the capability to analyze such complex systems over long time periods is uneven at best. In general, significant errors in performance assessment may occur due to the selection of the wrong deterministic model for specific phenomena, an incorrect analytical solution for the model, or an incomplete description of the system to be modeled.

In the case of the analyses of the behavior of some components, the refinement of the relevant models and the acquisition of additional data would permit significant improvements to be made. In other instances, the problem being analyzed may be essentially intractable given current analytical capabilities, or intractable within the time constraints under which the TSPA staff is operating. The distinction between those analyses that may be intractable and those that can be improved is important, because the approaches to deal with the two situations, as the project moves into the anticipated

TSPA-LA phase, are different. In Section III.D, approaches for dealing with the analyses that appear to be intractable are discussed. Improvements that can be made through updating the component models and the acquisition or use of additional data are discussed in Section IV.

D. Managing Complexities and Component Model Limitations

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; and
- 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.

As would be expected, the four identified approaches are closely related and, in fact, they are intertwined. Furthermore, the applicability of a given approach to a specific type of process will depend on the nature of the process. In the case of processes for which analytical models are available, significant improvements can be made through updating the component models and the acquisition and use of additional data. In the case of processes that may be essentially intractable, the only available option may be to treat them through the use of bounding analyses and/or design changes.

In contrast to the goal in the preparation of the TSPA-VA, the objective for the TSPA-LA should be to provide sufficient documentation so that it can be more readily defended as being either realistic or conservative. With these thoughts in mind, the Panel offers the following comments on the use and application of each of the identified approaches to these two types of processes.

Updating the Component Models

This approach primarily involves the improvement of the experimental and/or theoretical basis for the models. While, due to the physical size of the proposed repository and the temporal scale of the analyses, the site and design cannot be tested in a realistic manner, component models can be improved through refinements in the underlying subsystem models. At the same time, as the Panel noted in its Second Interim Report (Whipple et al., 1997), the capabilities of the project staff to analyze such complex systems over long time periods is uneven at best. In general, the performance assessment of complex systems may have significant errors if the wrong deterministic models are selected, if an inadequate or incomplete description of the system to be modeled is used, or if an incorrect analytical solution is applied.

Acquisition of Additional Data

Much can be accomplished through the development and acquisition of new data. This can be achieved through the conduct of well designed experiments, through observations and studies of natural analogues, and through analyses of other relevant systems in the field. All such steps can enhance the ability of the analysts to test the validity of existing component models and to increase their confidence in the estimates these models provide. Data that can be used to challenge the basic model formulations can be particularly useful. For example, data on ^{36}Cl collected during the site investigation imply faster travel of water in the unsaturated zone than was estimated using analytical models. Similarly, the modeling of transport has been revised in response to measurements of the groundwater transport of plutonium-bearing colloids at the Nevada Test Site. Additional discussion on this subject is provided in Section IV.

Bounding Analyses

Applications of bounding analyses generally produce results that are conservative. For this reason, the outcomes of such analyses are generally assumed to be highly credible by regulatory agencies. In addition, such analyses are commonly less data-intensive than those conducted on a more realistic basis. As a result, bounding analyses are particularly useful in cases where the existing analytical models have significant deficiencies that would be difficult and time consuming to correct. A good example of processes that fall into this category are those that are highly complex and extensively coupled. The application of bounding analyses would appear to be especially appropriate as the project staff approaches the preparation of the anticipated TSPA-LA. The chosen applications must, however, be defensible, and care should be taken to ensure that the performance of the systems to which the analyses are applied have only a minor effect on the results of the overall assessment. Otherwise, the use of bounding analyses may result in unacceptably conservative projections of the performance of the overall repository system.

That this can be the case was demonstrated in several instances in the preparation of the TSPA-VA. One example was the case in TSPA-95 (CRWMS M&O, 1995) where the analysts assumed that a waste package failed completely at the time of the first pinhole leak. For purposes of the TSPA-VA, a less conservative analysis was used to model this process. At the same time, it should be recognized that there were some issues for which the TSPA-VA was intentionally conservative. One example was the use of a bounding analysis to assess the risks from potential criticalities.

There are other cautions that should be observed in the application of bounding analyses. For a complex, non-linear system, it is not always readily apparent how conditions that bound performance should be defined. This makes it difficult to judge whether, and the degree to which, the generated results are conservative. Because of the difficulties inherent in developing fully-coupled models for analyzing the flow and transport in the unsaturated zone, it may prove advantageous to begin with a simpler set of models, and then to evaluate the more complex issues through either sensitivity studies or bounding evaluations. If these efforts demonstrate that certain aspects of the complex coupled phenomena can be ignored or treated one-dimensionally, the overall analysis will be vastly simplified. More effort, however, needs to be directed to defending this approach and ensuring that coupled effects, that are potentially detrimental to repository performance, are addressed in this manner.

Design Changes

As noted above, the incorporation of changes in the design of the repository system is suggested primarily as a means for addressing processes whose analyses are essentially intractable. Although this is not likely to be applicable to the processes affecting the transport of radionuclides in the saturated zone or biosphere, it does appear to be relevant to the analyses of the complexities associated with the coupled processes that occur as a result of the increased heat loading within the proposed repository. This is clearly a design issue. It is important to note, however, that the trade-offs between hot designs that delay water contact with the waste packages, versus cooler designs that may induce smaller changes in the natural system, are complex. The degree to which cooler designs are likely to be easier to analyze should be considered in the trade-off analysis.

Although the subject of changes in design is outside the scope of its charge, the Panel recognizes that there are other examples that might be considered. These include the possible use of backfill to avoid damage to the waste packages and other protective barriers by rockfalls. Again, however, this would likely result in higher temperatures inside the waste packages which, in turn, leads to a trade-off between protecting the waste packages or limiting the peak cladding temperature. Furthermore, such a design change is likely to lead to additional uncertainties in the chemical environment that will be experienced by the waste packages.

Concerns regarding the use of the results of the TSPA as a guide for making changes in the design of the proposed repository were discussed in Section II C.

Defense-in-Depth

As noted above, 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 fact, the viability of Yucca Mountain as a nuclear waste repository finally must rest on the evaluation of safety (expressed as some measure of radiation exposure to individuals or to a critical population). The TSPA is the primary tool for this evaluation; however, its inevitable complexity may obscure or even confound the safety analysis. For this reason, it is likely that, at the anticipated LA phase, the TSPA staff will be required to establish a fundamental safety case for the proposed repository. Developing such a case basically involves describing why and how the staff believes the repository could perform safely.

Accomplishing this goal is intimately involved with the defense-in-depth safety philosophy long used to provide an acceptable level of safety for other types of nuclear operations, that is to say, the analysts should take advantage of the use of redundancies in various barriers and systems to protect the public from being exposed at unacceptable levels. 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 (USNRC, 1998; CRWMS M&O, 1998e).

Conclusions and Recommendations

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. 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

E. Overall Conclusions about the TSPA-VA Methodology

The Panel believes that the basic framework or architecture of the TSPA-VA is sound, as is the use of abstractions of component models for purposes of computational efficiency. Where the Panel has concerns, it is more often due to the specific methods applied and the details of the component models, rather than with how the models are linked. In some instances, as noted in Sections II and IV, the Panel is concerned that inappropriately optimistic analyses may have been made.

In summary, the challenging features of the present TSPA-VA are that: (1) the already complex models are coupled; (2) the models are being extrapolated into temporal and spatial scales that are well beyond experimental data bases or human experience; and (3) there is little testing of the component submodels. Compounding the problem, there can be no test of the fully-coupled and extrapolated models used in the TSPA.

As summarized above, the TSPA-VA staff used a mixture of analyses, some of which were intended to be realistic, and others of which were intended to be conservative. For these reasons, and the limitations of the component models cited in Section IV, the Panel concludes that the TSPA-VA cannot be viewed as an accurate projection of the "probable behavior" of the repository.

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.

IV. COMPONENT MODELS OF TSPA-VA

A. The Unsaturated Zone under Initial Conditions

Three issues are addressed in Chapter 2 of the Technical Basis Document (CRWMS M&O, 1998c) on unsaturated zone flow: (1) estimating the infiltration rate and infiltration maps; (2) characterizing the hydrologic properties of the site; and (3) estimating seepage in the drifts under postulated (ambient) conditions. In general, substantial improvements over previous TSPA efforts are reported in all these areas. However, considerable uncertainties still remain.

Infiltration Rate

The infiltration rate, its variation in time, and to a lesser degree its variation in space (infiltration maps), are key variables to repository performance. Infiltration affects practically all other TSPA components and plays a crucial role on the rates of release of radionuclides and their transport in the unsaturated zone (UZ) and the saturated zone (SZ). It is also a key parameter in the characterization of the hydrologic and transport properties of the site.

Estimating the magnitude and the temporal and spatial variability of the infiltration rate is a difficult task. The issue is complicated by the fact that direct measurements of the infiltration rate are not available or easily obtainable (although there is anecdotal reference in the UZ expert elicitation report of a measurement of 50 mm/yr in the Exploratory Studies Facility). Therefore, infiltration rates, infiltration spatial maps and their variation in time are inferred in the TSPA-VA from indirect measurements or from mathematical models. Compared to previous reports, the TSPA-VA team has implemented a substantial change in its estimate of the current infiltration rate, which has been revised upwards by one order of magnitude. This change is a reflection of field evidence accumulated in recent years. The dramatic increase is consistent with the recent discovery of fast flow paths in the mountain, as evidenced by chlorine-36 findings. The revision has far-reaching effects, and has led to many qualitative changes in the conceptual models of flow and transport in the mountain. In particular, it has shifted the project's interpretation of flow and transport from predominantly matrix-dominated regimes to predominantly fracture-dominated (fast path) regimes.

In parallel with the revised estimate of a higher infiltration rate, the project also adopted a new approach for representing variation in precipitation in the base case by considering three substantially different climates of variable duration, dry (present), wet (long-term-average) and super-pluvial. The approach towards wetter conditions in the mountain, both present and future, is conservative and represents a drastic improvement over previous TSPA models, in which a constant (and much smaller) infiltration rate was used. At the same time, the climatic conditions for the base case and the postulated scenarios for switching between various climates are simply hypothetical and have large associated uncertainties (see also the related discussion of climate in subsection IV.K.).

Currently, the estimation of the spatial and temporal variability of infiltration is based on the use of water balance models at the mountain surface, coupled with hypotheses about future climates. Infiltration maps are computed from the models but are not directly measured. These models contain a number of simplifying assumptions on processes, such as precipitation, evapotranspiration, run-on and run-off, and on parameters, such as soil depth, flow dimensionality, etc. In the absence of experimental data to confirm these approximations, it is unclear how realistic they and the resulting infiltration maps are. 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.).

Hydrologic Properties

An accurate characterization of the hydrologic and transport properties of the site is essential for obtaining reliable predictions of the repository performance. Mountain-scale hydrology will influence the response to the thermal pulse, seepage into drifts, and the transport rates of released radionuclides. For example, it will provide the velocity fields to be used for flow and transport in the UZ during the life of the repository. The large disparity in the length scales involved, the intrinsic heterogeneity of the site, and the fractured nature of the mountain, however, present some difficult problems for the detailed characterization of the site. Ongoing efforts to address these problems through research are impressive and commendable, and although much is still unknown and/or uncertain, multiple advances have been made (Bodvarsson and Bandurraga, 1996).

Currently, the characterization of Yucca Mountain is based on a combination of experimental data from boreholes, laboratory measurements, pneumatic tests, air injection tests, field measurements and inverse computer modeling to estimate parameter values. The revised interpretation of infiltration has led to a more realistic and improved characterization of the hydrologic properties. Key findings include: the need for a substantial reduction in the fracture-matrix interaction in order to match saturation data under the revised infiltration rate; the observation of a strong anisotropy (ratio of order 10) between vertical and horizontal fracture permeabilities above the repository; the estimation of the capillary properties of the fracture continuum; and the identification of perched water zones. Using inverse modeling and matching of data to simulations, a set of parameter values has been obtained. They form the basis for the computation in the TSPA-VA of the key hydrologic aspects of the site, such as the flow fields, the saturation profiles, and the transport pathways.

Considering the complexity of the problem, the project has made many important strides. At the same time, significant uncertainties remain. The origin of these can be variously traced to the unprecedented scope of the problem, the novelty of some of the analytical problems involved, the inadequate representation of some physical processes, and/or the non-uniqueness inherent to inverse modeling. These uncertainties will propagate through many components of the report, closely linked to hydrology and transport, with significant ramifications on the final results. The Panel has singled out the following two areas, related to UZ flow in a fractured system and to inverse modeling, where additional advances will help increase the level of confidence on the TSPA estimates.

UZ flow in a fractured system

Determining UZ flow in a fractured system, such as at Yucca Mountain, involves the elucidation and representation of the process at different scales and geometries, such as a single-fracture, the interface between a single fracture and its matrix, the network of fractures, the matrix continuum and the interface between fracture continuum and matrix continuum. By necessity, however, the TSPA-VA approach is based on modeling the dual continuum of fractures and matrix, which is the simplest approximation that can capture the main macroscale (computational grid-scale) aspects of flow and transport in this complex geological setting. This approach is essentially a scale-up (an abstraction) of flow phenomena that occur over the multitude of smaller scales included in the respective fracture and matrix continua. Relevant issues that arise in this context include the representation of the flow and capillary properties at various scales and of the fracture-continuum/matrix-continuum interaction.

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 subgrid-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).

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.

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.

Inverse modeling

The extraction of the base case set of parameters in the TSPA-VA is based on matching the predictions of the DKM model to various data, including borehole data on saturations, by an inverse modeling procedure. The approach is novel, compared to previous work, and commendable. The complexity of the problem, however, requires that a large number of parameters (more than 150) be estimated from a small number of data sets (less than 300). In addition, various assumptions are introduced for computational or other reasons. For example, the assumption is made of strictly vertical flow and vertical variation in properties. This 1-D philosophy is also adopted in other components of the TSPA (such as the simplified description of thermohydrology). Although consistent with a strong anisotropy in some of the layers, this assumption may fail across stratigraphic discontinuities which favor lateral flow (as in the perched water zone). For certain sets of data, the inverse modeling involves matching of point values with the grid-block values of the upscaled variables of the DKM as discussed above. Given that the upscaling procedure is yet to be validated, such matching may not be meaningful. Several of these data have considerable uncertainties. Finally, in order to match the observed perched water zones with the results of the computer model, it was necessary to reduce the fracture permeabilities below the perched water zones by orders of magnitude. Whether this is representative of the true conditions remains to be demonstrated by field tests.

Coupled with the inherent non-uniqueness of the inverse modeling procedure and the questions on the realism of the modeling cited above, these approximations cast doubt on the validity of the obtained base case set of parameters. 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.

Seepage

Drift-scale hydrology critically affects the rates of canister failure, and thus represents a crucial component in repository performance. The current TSPA-VA incorporates, for the first time, a hydrological model at this scale for analyzing seepage in the drifts. This is a significant development. The analysis is based on the postulate that drifts are capillary barriers, which will retain infiltrating water until its saturation at the drift wall reaches a maximum value (of one) at which point seepage commences. The analysis is novel and informative. The TSPA-VA relies heavily on its predictions for estimating the fraction of waste packages contacted by seeps and the corresponding fluxes. Furthermore, sensitivity studies based on this model show this fraction to be the parameter with the highest sensitivity in terms of overall system performance. Thus, even though only recently investigated, this part represents a major component of the overall TSPA-VA effort.

The approach is based on steady-state flow in a fracture continuum and generalizes to heterogeneous media previous analytical work in the literature on homogeneous systems. The numerical analysis presented is innovative, emphasizing the important effects of correlated heterogeneity in creating early seepage and of the matrix-fracture interaction on transient infiltration pulses. In the TSPA-VA base case calculations, it is conservatively assumed that the matrix around the drift does not participate in the flow (which is equivalent to taking the fracture-matrix reduction factor equal to zero). One outcome of the calculations is the existence of a percolation flux threshold in the range of 2-3 mm/yr, which is of the same order of magnitude as the current infiltration rate estimate. For infiltration rates below this threshold, seepage is presumed not to occur. Another important estimate is that, in the base case, only 0.5% of the total infiltration will contact the waste packages.

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. For example, Figure IV-1 (Figure 3-13, CRWMS M&O, 1998d) shows that for a large range in the percolation flux, the variance in seepage fraction is large (and almost equal to its mean value). It is not surprising, therefore, that seepage into drifts is one of the most sensitive input parameters in estimating dose rate in the TSPA-VA.

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. The results from such investigations would also be useful to thermohydrology (TH) and thermochemical (THC) models that are to be used for assessing conditions during the thermal period.

2. Although recent experimental data are reported to be consistent with the seepage analysis, further testing is needed. A better characterization of the hydrologic properties near the drifts, an analysis of transient flow based on a discrete fracture network, and additional experimentation at the drift scale would test the model predictions and would help increase confidence on the TSPA-VA results. Efforts in these directions are currently under way.

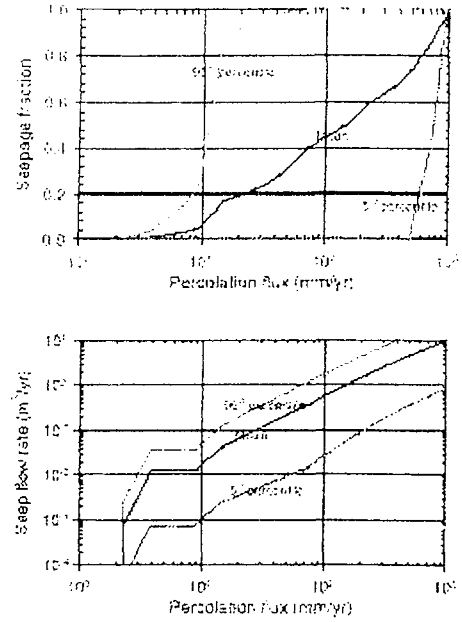

Figure IV-1. Calculated seepage fraction and seep flow rate as functions of percolation flux (Figure 3-13 of TSPA-VA).

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. As has recently been confirmed in the Large Block Test (Hardin, 1998), the possibility of episodic seepage events during the thermal period, as a result of instabilities, cannot be excluded. During the period of the thermal pulse, which is expected to last for several thousand years, thermomechanical and thermochemical effects on the permeability and capillary structure of the fracture network will alter seepage patterns as a function of time. In addition, drift collapse, as a result of thermomechanical or seismic events, will alter seepage patterns, rates and any accompanying contact of waste packages with water.

B. Thermohydrology

Background

The thermohydrology of the Yucca Mountain site is one of the most difficult aspects to analyze in developing an understanding of the behavior of the site as a potential repository for radioactive waste. The areal mass loading for the reference design is specified as 85 metric tons of uranium (MTU) per acre. This loading will cause a significant thermal disturbance in the repository environment for thousands of years after waste emplacement. The difficulties arise from the fact that the heat released influences the complex coupling between the hydrologic, chemical, and mechanical conditions that develop on different temporal and spatial scales.

The thermohydrologic (TH) processes occur at two important spatial scales: the near-field in the vicinity of the emplacement drifts (a few meters to tens of meters) and the far-field which encompasses the entire mountain (hundreds to thousands of meters). The near-field processes at the drift scale include thermal interactions within drifts and with the surrounding drift walls and floor. The far-field processes at the mountain scale include the influence of heat on liquid and gas movement above and below the repository. The thermohydrologic processes at both the drift and mountain scales affect fluid flow and transport in the unsaturated zone.

The evolution of the thermal pulse that will develop over time in the proposed repository has some interesting anomalies. These are shown by the vertical profiles on Figure IV-2 for the special case where there is an instantaneous emplacement of waste (Haukwa et al., 1998). At the repository level, the initial temperature is ~25° C, and it can be seen that after only ten years, temperatures at this level have increased to the boiling point for water at that altitude (~96° C). The boiling region expands above and below the repository because of heat pipe activity, and by 1,000 years, it can be seen that this isothermal zone of two-phase flow has reached a maximum vertical thickness of about 300 meters.

The cool down takes a much longer period of time because the thermal pulse can only be dissipated by the heat spreading out through the mountain, and this involves an enormous volume of rock. By 5,000 years, the boiling activity has ceased, but note on Figure IV-2 how the decreases in temperature above the proposed repository are offset by the increases in temperature below the repository. A comparison of the temperature profiles at 5,000 and 10,000 years shows how slowly the cool down process has become. Although the computed profiles shown on Figure IV-2 were obtained without considering the effects of thermohydromechanical (THM) or thermohydrochemical (THC) processes, the results can still serve as an indication of the basic factors that control the temperature field.

In the TSPA-VA conceptual model, the purpose of TH analysis is solely to provide information on waste package temperature, humidity and air mass fraction, as a function of time. This is then used as input for the canister corrosion model. The computation of the required quantities is done by a combination of hybrid models, without including any THC or THM processes. No other effect is included. Any alterations caused by THM or THC processes are assumed to be reversible. Further, it is assumed that the influence of the thermohydrologic processess would be short-lived, and therefore, "... thermal disturbances to seepage into drifts and radionuclide transport from the repository to the water table would only be important during the early period when no waste packages have failed, except for possibly a few juvenile failures." (CRWMS M&O, 1998c, p. 3-24.).

Coupled Effects

Substantial advances in the analyses of the effects of the thermal pulse on the Near Field Environment and Altered Zone (NFE/AZ) have been reported by Wilder (1996), Hardin and Chesnut (1997), and Hardin (1998), although these are not included in the TSPA-VA. For example, thermomechanical effects will result in a continuous change in the permeability of the fractures, and such changes will be irreversible in cases involving shear deformation. These effects will last as long as the mountain is heated or even longer. Rockfalls and roof collapse, induced by thermomechanical effects, will alter the temperature field inside and outside the drifts. Thermochemical processes will affect the permeability field as a function of time and they will alter the chemical composition of

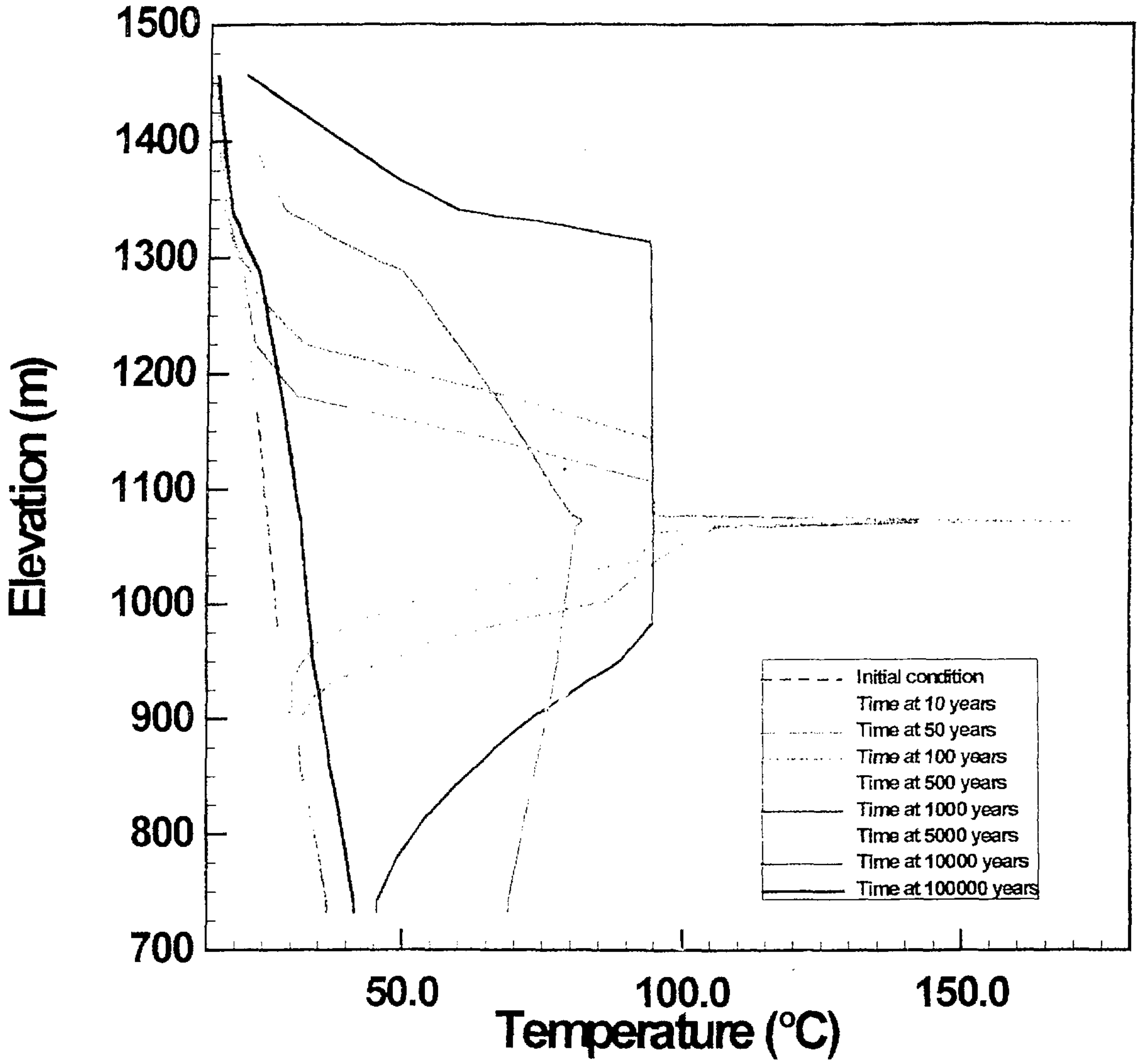

Figure IV-2. Simulated vertical temperature profiles at Yucca Mountain (from Haukwa et al, 1998).

the seeping water. In addition, thermochemical effects in the NFE/AZ may alter the sorption capacity of the formations below the repository.

A detailed and comprehensive analysis of how certain aspects of the THC processes affect the repository behavior is given in Chapter 5 of the Near-Field/Altered-Zone Models Report (Hardin, 1998). A critical component of the THC behavior is the impact of the heat pipe activity that, as can be seen on Figure IV-2, lasts for something between 1,000 and 5,000 years. Above the repository level, the temperature is projected to be sufficiently high to vaporize the water. This will occur primarily in the fractures and will leave a precipitate phase. The water vapor (steam) will move upward until condensation takes place in cooler spaces of the fractures. The condensate, being out of equilibrium with the rock, can dissolve mineral phases from the walls of the fracture, and the resulting solutions can migrate toward the heat source either by gravity (mostly in the fractures) or by imbibition (mostly in the matrix). Below the repository, the process is not completely the same because the liquids within the fractures, under the influence of gravity, can migrate away from the heat source and leave the two-phase flow system.

This dissolution of minerals at one point in the fracture network, and their redeposition at another could lead to the formation of a precipitate cap over the repository that varies in thickness as shown in Figure IV-3 (adapted from Hardin, 1998). The presence of the precipitate cap is indicated by the areas, primarily overlying the repository, where the fracture porosity ratio has decreased to 0.1 or less. For the base case, the initial fracture porosity at the level of the repository was taken as $\varphi_0 = \sim 10^{-4}$ (Hardin, 1998). Thus, the model results indicate that the fracture porosity of the cap has been reduced to $\varphi = \sim 10^{-5}$. Note that by 100 years time, the formation of the cap has started, and that by 5,000 years, the cap has reached its maximum thickness. This indicates that heat pipe activity continues well beyond 1,000 years.

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 affect the distribution and quantity of water flowing through the repository.

TSPA-VA Approach

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; the analysis by Hardin (1998) indicates these processes will persist over the life of the

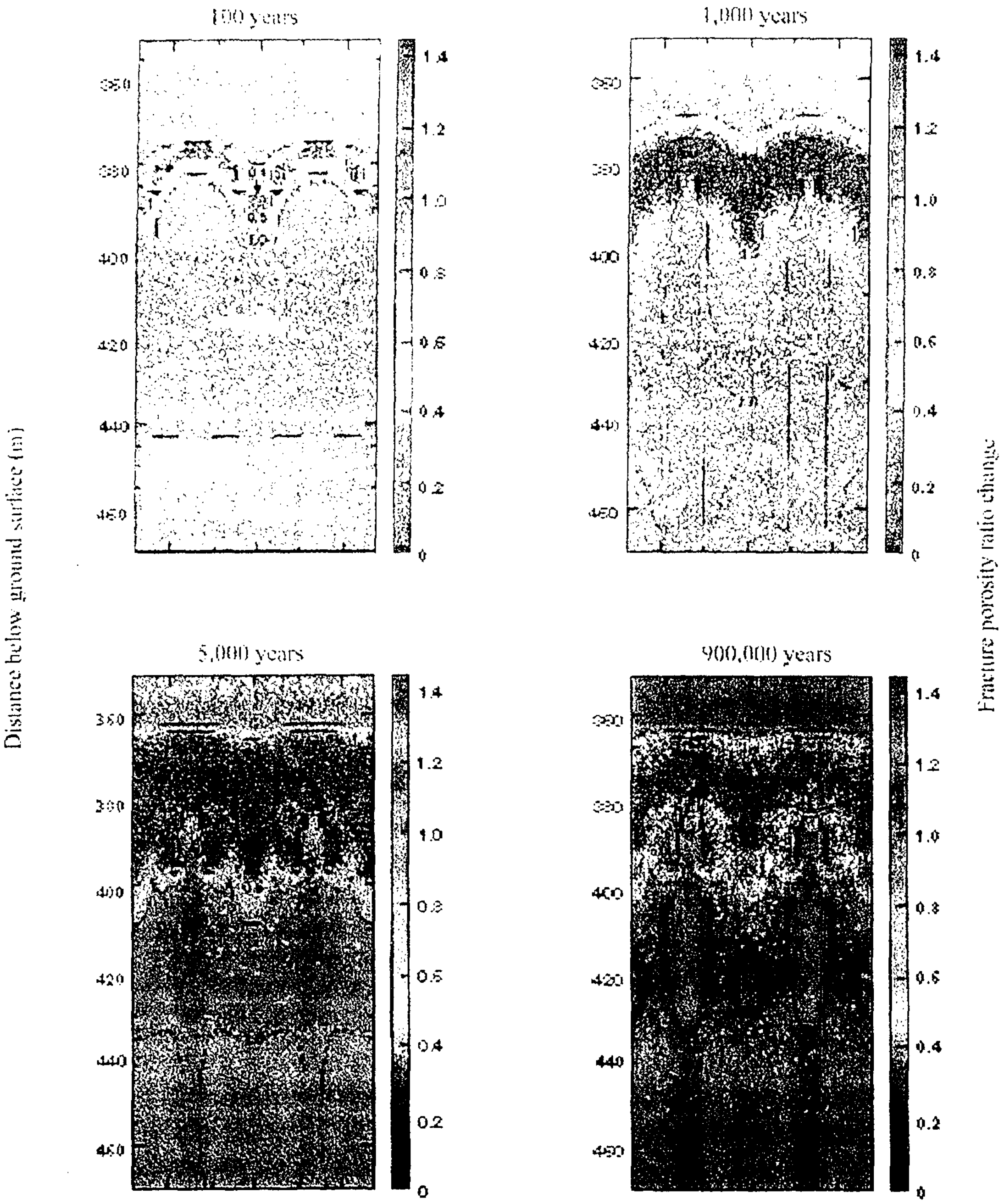

Figure IV-3. Development of precipitate cap over repository as indicated by fracture porosity ratio change (from Hardin, 1998).

repository. At the same time, as will be discussed below, 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 overpredicts 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.

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. During the thermohydrological period at Yucca Mountain, where phase-change conditions will prevail over long periods of time, there is an additional problem in fracture-matrix interactions as phase transformations occur in both the zones of boiling and condensation. Water vapor being generated in the boiling zone moves toward regions of lower temperature where condensation takes place. The way in which the condensate migrates back toward the heat source will depend on the fracture-matrix interaction. The thermochemical coupling referred to above will affect, and will be affected by, the way that condensate returns, namely whether it occurs primarily in the fracture or in the matrix. This problem is still unresolved, although some progress in this direction has been reported by Kneafsey and Pruess (in Hardin and Chesnut, 1997).

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 (CRWMS M&O, 1998a, p. 3-16). Whether this effect will be conservative or non-conservative is unclear at this point. Further study is needed.

   Related to this issue is the possibility that accumulated debris from the rockfalls in the drift can cover the waste package in such a way that there is a significant increase in canister temperatures during the thermal period. Depending on when the rockfalls occur as well as on their extent, the resulting waste package temperatures may exceed 350 °C, in which case the cladding may fail sooner than expected.

4. Thermochemical effects can be significant, particularly as far as the formation of a precipitation cap is concerned. Such a cap would affect the seepage predictions in the long term, as indicated in Hardin (1998), and can potentially represent a significant barrier to radionuclide releases. However, the analysis of this problem is still incomplete. In fact, its complexity raises the issue of whether the problem is analyzable.

   In addition to the previously cited matrix-fracture interaction during the period of heat pipe activity which will drastically affect the way chemical dissolution and precipitation occurs, we note some additional issues related to the flow of condensate in fractures.

   In the THC analysis that led to the development of a precipitation cap (Figure IV-3), it was necessary to evaluate the changes in porosity that would result from the deposition of minerals on fracture surfaces. The accumulation of such material would tend to reduce the fracture porosity and the permeability as well. The intrinsic permeabilities in the fracture and matrix continua were assumed to scale as the cube of the porosity. It was stated that this, "...is equivalent to cubic law if the fracture aperture is assumed to vary linearly with the porosity of the fracture continua." (Hardin, 1998).

   It is not at all clear, however, that these assumptions will hold. When one considers the heterogeneous conditions within the fractures and the fact that there are significant differences in the orientation of the three fracture networks (Sonnenthal et al., 1997) then the analysis of the migration of condensate under the influence of gravity may pose yet another indeterminate problem. The differences in the flows between fractures, whose orientations can vary from near-horizontal to near-vertical, will be one factor; and the fingering and meandering of flow paths within individual fractures will be another (Cook et al., 1990; Geller et al., 1998; Pruess and Tsang, 1990; Pruess et al., 1998; Pyrak-Nolte, 1987; Tsang, 1984). This raises basic questions as to how the nature of the buildup of material in the cap, at all locations over the repository, under such conditions can be analyzed.

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. However, no consideration was given to the THM effects, which will be caused by the expansion of the rock matrix as temperatures increase. The resulting increase in compressive stresses within this heated rock mass will, in general, lead to fracture closure and a decrease in permeability. Thus, 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.

5. Many of the questions raised can be (at least partly) answered from the results of the Drift Scale Test (DST), which is one part of the in situ thermal testing program (DOE, 1995) for Yucca Mountain. This test is an important experiment that will provide the first large scale underground investigation of the THM and THC processes which control the thermal behavior of the rock mass surrounding the proposed repository.

   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. A wealth of data and information will be gathered, especially much needed data for model calibration. An analysis of the results should be important to the critical problem of developing a basic understanding of the fundamental role of THM and THC processes in controlling the thermal behavior of the repository. Underground testing in fractured tuff on this scale has never before been performed. It is anticipated that the results will provide data that will lead to a reduction of uncertainties associated with these analyses. This will be important as DOE approaches the license application phase.

C. Near-Field Geochemical Environment

Background

The near-field geochemical environment (NFGE) is an important and complex part of the TSPA-VA analysis. The NFGE models the changing compositions of gas, water, solids and colloids within the emplacement drifts during the perturbed conditions of the post-closure repository environment. Although the NFGE provides a broad description of the chemistry within the drifts, it does not describe the corrosion environment directly in contact with the waste packages (e.g., crevice/pit corrosion environments).

The major perturbations to the repository drift environment are: 1.) the thermal period in which drift walls reach temperatures of several hundred degrees for periods extending for thousands of years, and 2.) the emplacement of large amounts of construction materials, e.g., steel and concrete, which react with the gas, water and solids of the repository. The thermal pulse not only increases reaction rates, but affects the movement of gas and water through the unsaturated zone. The emplaced construction materials can affect the compositions of gases and water during these reactions and the proportion and types of colloids.

It is within the near-field environment (which includes all materials and process which occur within the volume encompassed by the rock face of the drift) that far-field phenomena (e.g., infiltration rate and thermal-hydrologic processes) interact with the waste forms and waste packages (see Murphy, 1991, for a summary of the interactions). The near-field environment is the source term for the far-field environment. This coupling is well illustrated in the flow diagrams which link the information needs of the analysis to the process-level and abstracted models used in the TSPA-VA analysis (CRWMS M&O, 1998c, Chapter 4, Figs. 4-3 and 4-4). These diagrams not only emphasize the importance of the near-field environment (providing input for waste package degradation, waste form degradation and EBS transport), but also illustrate that the definition of the near-field geochemical environment (boundary conditions) depends critically on the site hydrology, site geochemistry, repository design, waste package design and the EBS design. The chemistry of fluids within this near-field environment set the geochemical boundary conditions for the corrosion rate of the waste package, cladding, UO_2 in spent fuel and vitrified waste, but the chemistry of corroding fluids is also affected by interactions with the waste package or waste forms on a smaller scale (e.g., within the waste package itself). The NFGE also determines the geochemical boundary conditions for the solubility limits of important radionuclides, the form of the radionuclides in the solution (dissolved species or colloids), and the types of radionuclide-bearing, secondary phases that may form.

All of the chemical and physical processes are highly coupled, and small changes in one part of the system may have large effects on other parts of the system. As an example, the thermally-driven dissolution, transport and precipitation reactions will affect the permeability and porosity of the repository rock in the near-field. This may change the fluid flow pathways into the drift with important effects on the seepage models used to describe the distribution of water on waste package surfaces. The project has provided a comprehensive list of the potential physical and chemical couplings (e.g., the analysis of interactions among gas, water and solid phases); but the extent to which these limited and loosely coupled models can represent the actual, coupled thermal-hydrologic-mechanical and chemical process in the NFGE remains highly uncertain. To quote from the project (CRWMS M&O, 1998c, Chapter 4, p. 4-4),

> The general TSPA model architecture is based on the ability to decouple system behavior both spatially and by type of process, (i.e., it assumes weak feedback spatially and among processes). This assumption is least tenable when applied to the NFGE, which may be highly coupled in a nonlinear fashion, being influenced by thermal, hydrologic, and multicomponent chemistry.

All of this said, the Panel notes that the actual level of knowledge of the near-field geochemistry that is required to describe waste package corrosion is much more limited, e.g., pH, chloride concentration, as discussed in Section II.C.

TSPA-VA Approach

The NFGE is represented by five sub-models (Chapter 4, 4-2): 1.) the description of gas, water and colloids as they enter the drift; 2.) the composition of the gas phase in the drift as a result of flow and chemical reactions; 3.) the evolution of water compositions as a result of reactions with materials in the drifts; 4.) the quantity and stability of colloids in the drift; and 5.) the development and effects of in-drift microbial communities. The connections (input/output parameters) of these five models to other models in the TSPA-VA are of critical importance in understanding overall results (Chapter 4, Fig. 4-4). Detailed comments on these five sub-models are given in Appendix A.

As an example, the flux of water into the NFGE is described by two models: 1.) The seepage flux model is used to describe the in-drift solid-water reactions and abundance of colloids; 2.) The average percolation flux is used for the in-drift gas model. The physical basis for using the two different models is the greater mobility of gas in the repository and the belief that the gas phase will be in equilibrium with the larger volume of water present over a wider area of the repository. Further, the thermal models provide additional input parameters for the NFGE: 1.) flux of gas into the drift; 2.) drift temperature; 3.) relative proportions of air and gas in the drift. The movement of water and gas through the repository is highly dependent on permeability which can change as a result of dissolution, transport and precipitation reactions in the near-field. These important thermal-hydrologic-chemical couplings are not, in fact, incorporated into the models used in the TSPA-VA, although side analyses of these effects are considered (Hardin et al., 1998). A good discussion of the connections of the NFGE to other models in the TSPA-VA is found in Chapter 4 (Section 4.1.2.1).

General Findings

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.

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.

However, the project should realize that even if the necessary fundamental data can be obtained and increasingly sophisticated models are used in the analysis, the uncertainty in the NFGE models may continue to be large. The causes of these large uncertainties have been discussed by project scientists (see CRWMS M&O, 1998c, Chapter 4, pp. 4-13 to 4-17). Some, but not all, of these causes include: (1) site heterogeneity and its evolution over time, (2) the coupling between thermal and chemical processes and resultant refluxing will have a substantial impact on the near-field hydrology; (3) water compositions are profoundly affected by the gas phase assumed to be in equilibrium with the evaporating water, and this in turn depends on whether the system is modeled as being open or closed; and (4) cementious materials which undergo thermally driven phase transitions. 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.

In principle, successful geochemical models of the near field environment will require (Bethke, 1996):

1. All principal components must be identified and for fluids their fluxes determined.
2. There must be thermodynamic data for the important species in the system. In the case of the Yucca Mountain project, this question should be specifically addressed for the uranium and other radionuclide phases.
3. The equilibrium constants for the important reactions in the thermodynamic database must be sufficiently accurate for the model requirements.
4. The activity coefficients of relevant molecular species must be calculated accurately.
5. Kinetic rate constants for principal reactions must be known. Although the consideration of kinetics is important to the development of the conceptual models, this can introduce considerable uncertainty into the analysis. The most important difficulty will be in relating experimentally measured rate constants to reaction rates in nature (see for example, Carroll et al., 1998).

6. Geochemical systems often fail to reach equilibrium, thus it is important to determine which reactions may in fact reach equilibrium.

7. There must be enough experiments with the principal components of the system over the range of relevant conditions to determine whether the important reactions used in the models have been identified.

We expect that it will be difficult to provide full and satisfactory answers to each of these questions (and this is not a criticism of the project). We also expect, however, that even partial answers to the above questions will require a major experimental effort integrated with field tests and studies of natural systems. In the absence of such an effort, the near-field geochemical models will remain highly speculative with large uncertainties.

We emphasize this point with quotes from the overview description of the NFGE (CRWMS M&O, 1998c, Chapter 4, 4-3):

> A number of major aspects of the NFGE are shown schematically within Figure 4-1, but a full description of the near-field geochemistry is not currently possible.

The Panel notes that even after considerable effort the resulting incomplete description of the NFGE may still contain large uncertainties.

Throughout the TSPA-VA, sensitivity analysis is proposed as a method by which the range of important parameters and phenomena might be reduced and as a means of reducing uncertainty. This is probably difficult to do effectively for the models used in the NFGE. Sensitivity analysis of important parameters cannot be used in place of experimental studies of the actual, relevant, coupled, geochemical phenomena.

The project itself notes (CRWMS M&O, 1998c, Chapter 4, page 4-78) that,

> Much of the uncertainty for the NFGE stems from conceptual model uncertainties. This is particularly true for models of in-drift materials that use thermochemical data(equilibrium and kinetic parameters). The coupling among geochemical effects and physical processes in real systems cannot be incorporated comprehensively into the current NFGE models. The inability to represent this coupling is another large contributor to conceptual uncertainty in these models; this is particularly the case for the evolution of the gas composition in this system.

Finally, the Panel notes that a detailed review of the NFGE is beyond the scope and time constraints of this Panel, although specific comments are made in Appendix A. A detailed review would require careful consideration of the actual values used or generated by sub-models and a judgment as to their appropriateness and consistency. A proper review will require many parallel geochemical calculations using several of the generally available geochemical codes and databases. 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.

D. Waste Package Degradation

Overview of Waste Package Performance

Based on the TSPA-VA results, the project analysts have judged that the rate of waste package degradation will be a principal determinant of overall repository performance. Hence the integrity of the waste package as a barrier is critical to the performances of the repository as projected within the TSPA-VA for each of the time periods considered: 10,000, 100,000 and 1,000,000 years (CRWMS M&O, 1998d, pages 0-16). Since corrosion has been deemed to be the most important factor that might accelerate the rate of such degradation, the TSPA-VA staff focused on this process, specifically as it relates to the performance of the various metals that are under consideration for the waste package. These efforts, which the Panel supports, have led to significant progress in the development of models for the analysis of localized corrosion in corrosion resistant metals (CRM), such as C-22 and titanium, and of more general corrosion in metals, such as carbon steel. However, much work remains to be done. Included in the discussion that follows is a summary of the status of certain key subject areas, followed by an identification of several important areas in which research is needed.

Crevice Corrosion

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.

In anticipation of the development of the TSPA-LA, it will be necessary for the project staff to demonstrate whether crevice corrosion will persist under the realistic environments anticipated within the proposed repository. In short, the crucial issue is whether CRM will resist localized corrosion in the realistic range of repository water chemistries and temperatures and the anticipated frequency of wetting of the waste canisters over long periods of time. If C-22 remains passive, the anticipated corrosion rates will be extremely slow and canister life prior to penetration is projected to be thousands of years. The important issue is the amount of corrosion damage that occurs to waste packages that are within the critical temperature range, when the processes leading to crevice corrosion will be promoted. Significant influencing factors are the time at which a waste package surface temperature cools to within this critical range, the time it remains within the range, and the time at which the waste package cools below the critical range. Once outside the critical range, the waste package will no longer be susceptible to crevice corrosion.

Once the surface temperatures of the waste package are within the critical range for the promotion of crevice corrosion, the controlling factor will be the chemical composition of waters in contact with the waste package metals. In this regard, the chemical nature of the water that will determine its corrosion characteristics is likely to be determined more by processes at the waste package surface than by those taking place at the drift wall and in the surrounding rock. Reactions at the metal surface, under deposits, and within crevices, will significantly change the water composition. Both metal-nonmetal crevices (and the accompanying corrosion products, deposits, rock and debris), and metal-metal crevices, are of concern. One of the outgrowths of the TSPA-VA was a documentation of the significance of the chemistry of the water in contact with the waste package surface. The Panel recognizes this contribution to the understanding of this matter. 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.

Stress Corrosion Cracking

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. This is especially true in light of the tentative nature of the models and treatment of SCC. At this point, the analysis of SCC of C-22 is a work in progress. Adding to the uncertainties is the fact that this failure mode is closely coupled to waste package fabrication procedures. These include the processes for welding and shrink-fitting the canisters. Compounding these uncertainties will be stresses from any deformation during placement or brought about by rockfalls, and any movement of the canisters subsequent to placement. In the case of the TSPA-VA, the Panel has concluded that the 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.

Analytical Needs

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. The outcome of such efforts will be closely coupled to other important processes and will describe important parameters, including (1) the time sequence of waste form exposure to the repository environment, (2) the transport of water and other species into the waste packages, and (3) the release and transport of radionuclides from the waste packages.

In terms of analyzing the potential effects of rockfalls, the development of the required mechanical models are reasonably well in hand. The same is true in the case of models for analyzing the corrosion of steel under dry and wet conditions. 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 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.

Research Needs

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.

The research needed to answer these types of questions are but one example of the challenges in this area. As with any such analyses, the use of appropriate and relevant data is crucial.

Base Case and Alternate Designs

The selection of design alternatives for evaluation in the LA, assuming the project reaches that stage, is a work in progress (Enhanced Design Alternatives (EDA) Workshop, Jan 4-15, 1999). Included in this effort is an evaluation of alternative designs for the waste packages. Several design concepts are under consideration, including large waste packages composed of steel/CRM combinations, large waste packages composed of CRM/CRM combinations, and smaller packages composed of CRM alone. Pertinent to the decision-making process is that large waste packages require thick walls to comply with the design requirements for dropping and tip-over during manufacture, handling, transportation, and emplacement.

The base case design is a large, steel/CRM waste package that includes a 10-cm outer barrier of steel over a 2-cm inner barrier of alloy C-22. Concerns regarding the use of steel include a relatively high corrosion rate during wet periods, the potential effects of the ferric ion from the corrosion of steel on the corrosion of the CRM layers, and the effects of the relatively voluminous amounts of iron oxide corrosion products. For these reasons, steel has been eliminated from some alternate designs; only corrosion resistant metals are used. Various layers and thicknesses of C-22, titanium and other corrosion resistant metals are included among the design options.

Among the issues that arise are:

1. A steel outer canister provides mechanical and shielding benefits but lacks corrosion resistance. Steel is strong, ductile, tough and readily fabricable. Under hot/dry

conditions, it oxidizes at a moderately low rate. However, under moist conditions (approximate relative humidity ≥ 60%), the corrosion rate is substantial; under dripping and wet conditions, it is even more rapid. The result is that steel does not offer much long-term protection after any dry-out period is over. For a given package, penetrations of 10-cm steel can occur in as little as tens of years if wet conditions persist. The times to penetration will be longer if wet conditions are not continuous.

2. CRM waste packages without steel have superior corrosion resistance. Several alternative designs consist of single and multiple layers of C-22 and titanium. Both of these metals have excellent corrosion resistance in oxidizing solutions and the nominal environments anticipated in the proposed repository. Corrosion penetration rates for metals in the passive state are on the order of a micrometer per year or less. If these corrosion rates pertain, waste package lives of 10,000 years or more per centimeter of CRM are projected, even if the waste packages are continually wet.

3. A steel inner canister, within a CRM outer canister, provides mechanical and shielding benefits and is protected from corrosion by the CRM. If the CRM remains passive in the repository environment, a waste package of this design is projected to have a long life. Should the CRM canister fail by localized corrosion, the likely path for moisture to the steel would be through a small pit or a tight crack in the corrosion resistant metal. The transport of moisture and oxygen through the penetration will control the corrosion rate which, for steel, is much lower under conditions of restricted oxygen transport as contrasted, for example, to surfaces that are freely exposed. While more detailed analysis is required, it is likely that the corrosion rate would decrease significantly with time.

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. The processes and events identified in the TSPA-VA are relevant to all of the designs. The process models, analyses and data for the TSPA-VA are also relevant. The same data needs pertain for each of the design options, i.e., the determination of the ranges of realistic water compositions and the determination of the corrosion performance of metals, e.g., C-22, titanium, 825 and 316 L, in the anticipated repository environments. The research needs identified throughout this section are meant to illustrate the types of data that will be required to support the selection of a final option. A rationale, supported by analysis and data, is required for the specification of metals (both sequence and thickness) for the waste packages.

Significance of No Backfill

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. Backfill can have multiple, coupled, and complex effects on the analysis of waste package behavior. It can, for example, protect the waste packages from damage due to rockfalls, and it will have a significant influence on certain conditions, such as temperature and relative humidity. Over shorter time periods, backfill can change the chemical composition of waters entering the drifts. However, its ability to change the long-term chemical composition of waters from the ambient conditions is questionable. 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.

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 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 titanium or C-22 – fabrication and durability. 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.

Environmental Conditions At, On, and Within the Waste Packages

As noted previously, the amount, distribution, and composition of waters within the drifts, and in contact with the waste packages, will have a profound impact on their behavior. In fact, the corrosion behavior of the CRM is controlled by three important properties of these waters, namely, their (1) concentrations of ionic species, (2) acidity (pH), and (3) oxidizing potential (Eh). The chemical and electrochemical processes that can alter these properties include (1) increased concentrations of dissolved chemicals in water and the formation of deposits on hot surfaces, (2) the formation of new corrosion products, (3) interactions with prior corrosion products previously formed, and (d) oxidation and reduction reactions taking place as part of the corrosion process. In addition, radiolysis can alter solution chemistry and generate oxidizing species which increase the Eh. Microbiological activity can also alter the solution chemistry, and galvanic action between dissimilar metals can affect corrosion processes.

On the basis of its review, the Panel offers the following observations:

1. The ambient waters at Yucca Mountain are innocuous to CRM. From the perspective of the corrosion of CRM, changes in the chemistry of the incoming waters that occur within the EBS, including those at the drift wall, and, in particular, on the waste package surfaces, are far more important than those that occur outside the drifts due, for example, to thermal hydrological effects. In the latter case, the waters remain innocuous. In contrast, reactions at the metal surface, under deposits and within crevices, can lead to significant changes in water composition. Of most concern are metal/nonmetal crevices with corrosion resistant metal and corrosion products, deposits, rock and debris, and metal/metal crevices involving C-22/steel, C-22/C-22, C-22/Ti. The Panel is aware that increased experimental work is underway in this area.

2. 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. What is the critical temperature range? When are metal

surfaces within this temperature range? What is the wetness (water seepage) during this period? Is there backfill present? Are there prior corrosion products? What is the condition of the liner and drift wall? Are rock and debris in contact with the waste package

3. As noted above, the effects of backfill on moisture flow to the waste packages and radionuclide transport from those that are damaged are complex. At the present time, the corrosion behavior of the waste packages with backfill or rock debris covering the waste packages is not well defined. Intentional backfill, rock and concrete debris, calcareous deposits and precipitated salts, and corrosion products will all affect the composition and distribution of waters in contact with the waste package. Without backfill, the waste package/engineered barrier system is likely, after a few hundred years, to be covered by rock rubble, calcareous deposits and precipitated salts, and corrosion products. It is important to recognize that the waste package surfaces will be covered and water droplets are not likely to impact surfaces directly, but rather water will move by film flow. Where particulate matter covers the metal surfaces, they may be saturated or unsaturated depending upon the amount of water.

4. 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. One approach would be through the preparation of a white paper detailing the accompanying analysis. In addition, the analyses of radiolysis and its effects on alternate waste package designs need to be documented. This should include information of the radiation flux as a function of material, thickness and time.

5. The study of microbiologically influenced corrosion (MIC) has been a continuing activity in the waste package degradation program. MIC is not a different mechanism or form of corrosion; rather it represents a process that affects uniform and localized corrosion processes through alteration of the environment. The TSPA-VA staff has determined that microbes and nutrients that could support MIC are present at Yucca Mountain (CRWMS M&O, 1998c, Chapter 5.). However, the likelihood of the formation of a sustainable biofilm on the waste package metal surfaces has not been demonstrated.

   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 WP 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 (CRWMS M&O, 1998c, Chapter 5), 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 (CRWMS M&O, 1998b.). The project staff has provided no documentation that MIC will increase CRM corrosion rates beyond the current range of uncertainty.

6. Galvanic action, due to the contact of dissimilar metals in a common environment, can significantly affect corrosion through the polarization of the metal surfaces to more oxidizing conditions for the more active member and more reducing conditions for the more noble metal. For the proposed repository, a likely galvanic couple for the base case WP design is between steel (more active) and CRM (more noble). The conclusion of an expert elicitation (CRWMS M&O, 1998b) was that galvanic action would have little effect on the corrosion of either corrosion resistant metal or steel. This conclusion was based on the expected geometry of the galvanic couple on waste packages and the presence of prior corrosion products. Based on its review, the Panel agrees with this conclusion.

WAPDEG and Individual Corrosion Models

Analyses of waste package degradation in the TSPA-VA were accomplished through application of the waste package degradation (WAPDEG) model. Within this model, the treatment of corrosion is developed to a level of complexity that extends well beyond the data that were available. The ability to consider this level of complexity may be useful for the LA phase if sufficient data on key parameters become available. If not, attempts to apply this model may compromise the transparency of the treatment.

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. The modular format for various degradation processes and the decision-tree flow through the model are useful, but the existing version of this model misses some important degradation processes that are not being adequately addressed. In particular, the model, as used in the TSPA-VA, did not prove to be well suited for analyzing designs other than those in the base case. In addition, the model is "hard-wired" and this restricts the flexibility for conducting certain sensitivity studies. Nonetheless, realistic aspects of the physical, chemical and electrochemical behavior that can affect the waste packages are generally treated in a clearly stated and rational manner. 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.

Complexity of WAPDEG Model

The complexity of the WAPDEG Model for waste package degradation is illustrated in Figure IV-4, the WAPDEG Model Logic Diagram. One of the characteristics of this model is that it incorporates a series of individual corrosion submodels that are organized

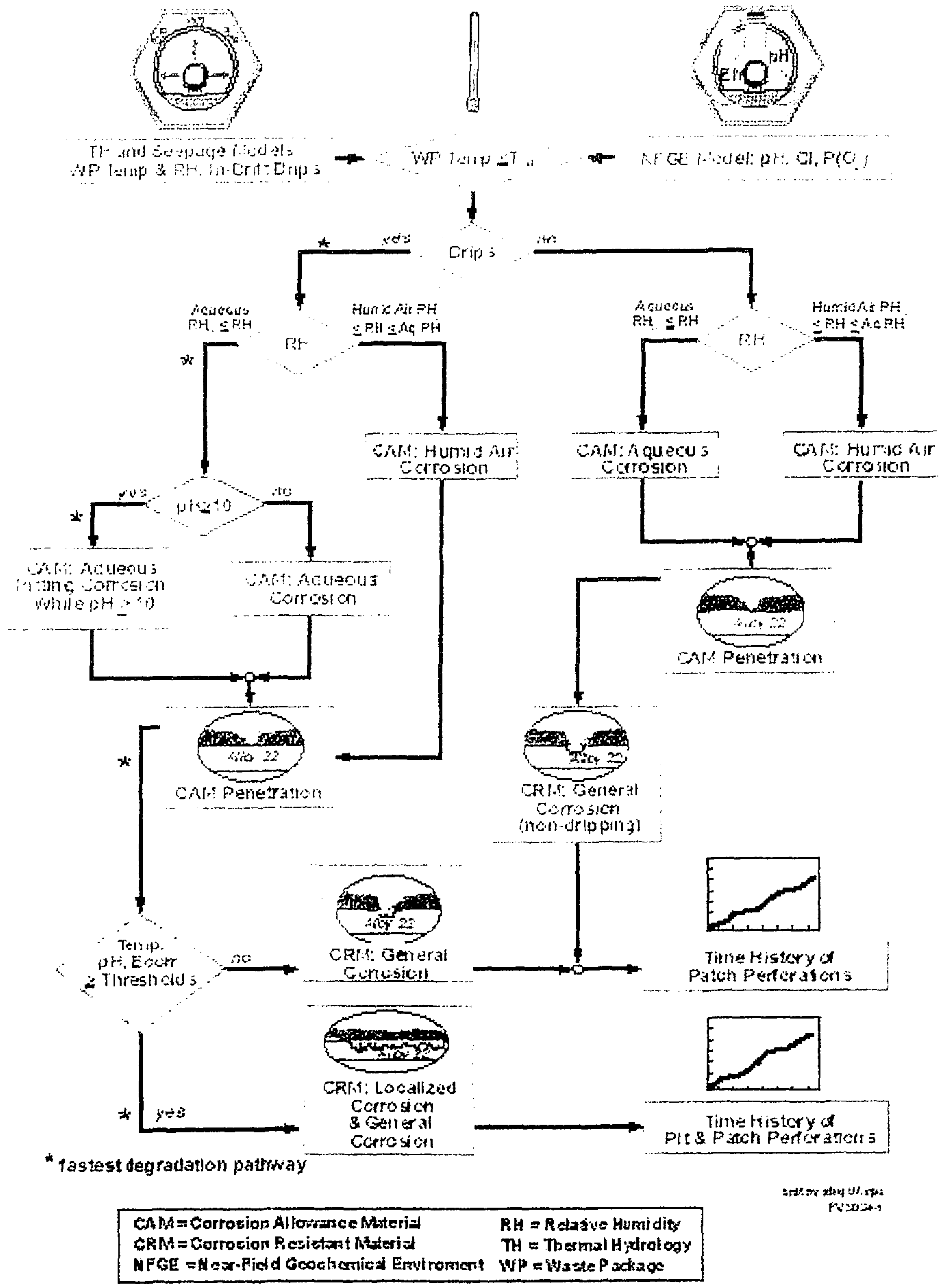

Figure IV-4. Logic diagram for waste package degradation model (Figure 3-44, TSPA-VA).

in a decision tree mode. These are designed to analyze the corrosion behavior of steel, a corrosion allowance material (CAM), and C-22, a corrosion resistant material (CRM), respectively. The cumulative depth of penetration for the outer steel barrier is determined through a series of time steps. When the total penetration within a patch equals the outer barrier thickness, the inner barrier of CRM is assumed to be exposed to the environment and the CRM models are then used to estimate the cumulative penetration of this barrier. 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.

There are advantages and disadvantages to the complexity of the WAPDEG model. Among the advantages are that it has the potential for more realism in the analyses, and that it permits flexibility in the treatment of processes that have spatial and temporal changes. The complexity of the model will also provide the option for flexibility in treating additional aspects of corrosion behavior. This will be especially true as additional data are obtained and the understanding of the TSPA analysts improves. At the same time, however, the WAPDEG model has clear disadvantages. These include a loss of transparency, difficulties in tracking the decisions and assumptions made and the impacts of these on model outputs, and an increase in the need for supporting data and knowledge that may not be available (or may not be obtainable). In addition, the complexity associated with the model can mask uncertainty.

Another problem is that the results and output of the analyses are not straightforward or direct with respect to the understanding of a typical corrosion rate vs. time behavior for a wetted patch in a selected environment. 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.

Analysis of Corrosion

The information needs for the individual corrosion models within the WAPDEG model are identified in Figure IV-5. These needs include information regarding the environment (e.g., temperature, relative humidity, pH and Eh), and information regarding the corrosion behavior of the metals (e.g., critical temperatures for localized corrosion, and corrosion rates over a range of conditions). Because of a lack of data for the various input parameters, the TSPA-VA staff depended to a large extent on expert elicitation. The

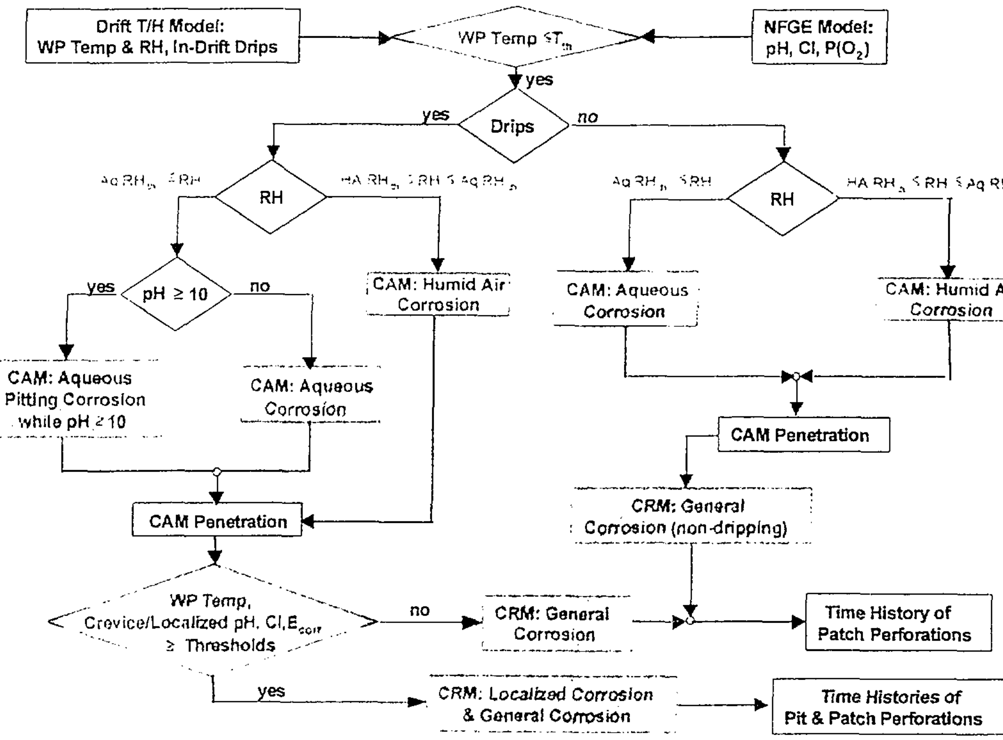

Figure IV-5. Information needs for the waste package degradation model-WAPDEG (Figure 5-5 Chapter 5 of Technical Basis Documents).

Estimates for WAPDEG that were based on Expert Elicitation are shown in **Boldface.**

Condensed moisture sufficient to support corrosion:

T_{TH} = Temperature threshold for moisture on WP to support aqueous corrosion

Relative humidity threshold for humid air corrosion of carbon steel:

HA RH_{TH} = Relative humidity threshold for corrosion of carbon steel

Relative humidity threshold for aqueous corrosion of carbon steel:

Aq RH_{TH} = Relative humidity threshold for corrosion of carbon steel

Critical pH for pitting corrosion, versus general corrosion, of steel:

pH > 10 = critical pH for pitting corrosion of carbon steel

CAM aqueous pitting corrosion: Pit Rate = $B \cdot (\text{time})^n$:

B = constant in pit growth law for carbon steel;

n = time constant in pit growth law for carbon steel

CAM aqueous corrosion:

Corrosion rate of carbon steel with drips

CRM general corrosion/no drips:

Corrosion rate of CRM, non-dripping

CRM general corrosion/with drips:

Corrosion rate of CRM, with drips

CRM localized corrosion:

pH and Eh of 3 Realistic environments: moderate, harsh and severe

% distribution: fraction of WP's in each of three environments

T_{CRIT} = critical temperature for localized corrosion in each of 3 environments

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.

Discussed below is the application of the WAPDEG model to corrosion resistant and to carbon steel materials.

Corrosion Resistant Materials

The output of the corrosion model for the analysis of CRM is a failure distribution for two conditions: (1) a waste package that is wetted all the time and (2) a waste package that is never wetted. These distributions become part of the information flow for probabilistic sampling in the TSPA realization runs. For purposes of these analyses, the waste package surface is assumed to be divided into over 900 individual patches, each measuring 310 cm^2 in area. The analysts assume that, if the waste package is dripped on, all patches are affected, and that they are wetted continuously throughout the period of analysis. Although the patches are identified as being on the top, bottom and sides of the package, no distinction is made for the location of the corrosion. It is also assumed that the CRM corrodes passively. Although a different corrosion rate distribution is assigned to wet and dry patches, both distributions are based on expert elicitation. Localized corrosion of wetted patches is assumed to lead to pitting, and localized corrosion of dry patches is assumed to lead to "patch" failure, that is, the entire patch is penetrated.

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.

Carbon Steel Materials

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.

One aspect of the analysis that may be non-conservative is the failure to consider the exposure of steel to thick, moist particulate matter (sand, debris or corrosion products). Steel in moist sand can corrode more rapidly than steel that is fully immersed in water or in water saturated sand. The corrosion of steel is controlled by the availability of oxygen to the wetted steel surface; corrosion rates are much lower for conditions of restricted oxygen transport.

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.

Waste Package Sensitivity Analyses

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 (CRWMS M&O, 1998d, Section 5.4). 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. Although sensitivity analyses are discussed in another section of this report, additional comments relevant to waste package issues are presented here.

The impact of the general corrosion rate of C-22 under dripping conditions is evaluated in a sensitivity case within the TSPA-VA packages (CRWMS M&O, 1998d, Section 5.4.1). 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 experts (CRWMS M&O, 1998b.) 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.

Two sensitivity cases analyzed in the TSPA-VA dealt with the moisture flow by drips (CRWMS M&O, 1998d, Section 5.4.2) and the pattern of seepage into the drifts (CRWMS M&O, 1998d, Section 5.4.3). 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.

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 (CRWMS M&O, 1998d, Section 5.4.4, Vol 3); the other was the presumed impact of microbial activity, which can lead to changes in water chemistries and possibly increased rates of corrosion (CRWMS M&O, 1998d, Section 5.4.5). 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 designs (Enhanced Design Alternatives (EDA) Workshop, Jan 4-15, 1999). 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.

Physical Events and Processes

Throughout this section, 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. The resulting expansion in volume (up to a factor of two) due to the corrosion of steel was not analyzed in the TSPA-VA. Such expansion can spall coatings and deform materials in contact with the steel. Growth of the corrosion products between the steel layer and the corrosion resistant layer can deform the CRM.. This is similar to the phenomenon of "denting" in the steam generators in pressurized water reactors and to "pack-out" of structural steel beams. Consideration of the likelihood and effects of this phenomenon is required when steel is used as either an outer layer or an inner layer of the waste package.

2. Insufficient treatment of fabrication and placement effects. This adds to uncertainty. Procedures used in welding, heat-shrink fitting in assembling the canisters, in supporting the canisters on pedestals, and associated fabrication activities, can have significant effects on corrosion and performance. Welding produces chemical and microstructural heterogeneities within the canisters, and the residual stresses from welding will approach the yield stress of the metal in the as-welded condition. Shrink fitting results in an uneven crevice between canisters; this increases the residual stresses. Waste package supports of steel can produce crevices that can trap moisture. The effects of corrosion and subsequent collapse of these supports are undetermined.

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. Intentional backfill, rock and concrete debris, calcareous deposits and precipitated salts, and corrosion products will all affect the composition and distribution of waters in contact with the waste package. The waste package surfaces will be covered. Although water droplets are not likely to impact surfaces directly, the water will move by film flow. Where particulate matter covers the metal surfaces, the local environment may be saturated or unsaturated depending upon the amount of water.

   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. The corrosion of steel is controlled by the availability of oxygen to the wetted steel surface, and the corrosion rates are likely to be significantly higher than that for immersed conditions. 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.

4. Corrosion of steel beneath CRM . For a waste package design with outer CRM and inner steel barriers, the TSPA-VA analysis is likely to be highly conservative and will overstate the corrosion rate of steel. Should the CRM canister fail by localized corrosion, the likely path for moisture to the steel would be through a small (pit) or a tight (crack) in 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.

5. Incomplete status of the analysis of stress corrosion cracking of C-22 and other Ni-Cr-Mo alloys. The performance of the alloys is a function of their metallurgical condition and tensile stress state, as well as the environment. Further analysis and experimental data are needed in support of the analyses of these effects.

Data and Related Research Needs

The experimental data and research needs noted throughout this section are itemized here. 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. These characteristics include: temperature, pH, Eh and ionic concentrations (Cl, SO_4, NO_3, CO_3, Fe^{+++}, Ca, etc.). For purposes of the analyses to date, two sets of presumed environmental conditions have been suggested. The first of these were an outgrowth of the Waste Package Expert Elicitation (CRWMS M&O, 1998b). This group suggested the following: moderate-pH 3-10; harsh-pH 2.5 and Eh 340 mV; and severe-pH 2.5 and Eh 640 mV. The second set of guides was an outgrowth of a waste package materials workshop. This group suggested that two types of water be assumed: (a) a J-13 type water that is relatively benign for corrosion of CRMs; and (b) a pH 2 acid, chloride-sulfate-nitrate water which is more aggressive. Ultra-aggressive environments, such as concentrated ferric chloride, were deemed to be unlikely and unrealistic under the anticipated repository conditions (Workshop on Waste Package Materials Testing and Modeling, May 7, 1998, Las Vegas, NV). While the suggested conditions proved useful in guiding preliminary discussions of the selection of canister materials, participants in both groups emphasized that a more rigorous determination of water chemistries will be required in support of upcoming analyses.

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. In undertaking this task, the ensemble of properties and species need to be considered as a whole; no single property or species should be evaluated in isolation. For example, it is not realistic to consider chloride ion effects alone; mixed chloride, nitrate, sulfate effects are more realistic.

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.

4. Determination of the lowest temperature at which crevice corrosion can continue (T_{CREV}). This temperature is a critical factor for materials selection and performance assessment. At temperatures below T_{CREV}, the metal will remain passive, and crevice corrosion will not occur. The value of T_{CREV} is a function of both the corrosion resistance of the metal and the chemical composition of the environment. A more corrosion resistant metal has a higher T_{CREV}; a more aggressive environment will reduce the T_{CREV}. The values of T_{CREV} for the extreme boundaries of water compositions need to be determined experimentally. The Panel recommends that alloys such 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.

5. Determination of the corrosion resistance of titanium. Embrittlement by hydrogen is the most important concern with respect to the corrosion of titanium. The relevance of two situations to repository conditions needs to be determined: (1) titanium in contact with carbon steel; or (2) titanium in hot, alkaline solutions. The fluoride ion is present in the repository waters and can be aggressive to titanium. The Panel recommends that the likelihood of corrosion due to fluoride be evaluated. In pursuing this task, however, this analysts should consider the effects of mixed-ion solutions, because the fluoride ion will not occur in solution without other anions and cations being present.

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). A realistic range of values for the penetration rate of metals (in the passive state) is required for determination of penetration times for the waste packages. The morphology of corrosion damage and penetrations in the waste package are needed to estimate the transport of radionuclides and to assess the anticipated performance of the repository.

7. Determination of the stress corrosion 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.

8. Elucidation of the effects of fabrication and emplacement procedures on waste package performance. Issues such as welding, shrink fit, pedestal material and geometry were not addressed in the TSPA-VA. They should be addressed in the LA.

9. Conduct of short term corrosion and electrochemical tests. These are needed to support the conceptual behavior and process models for localized corrosion.

10. Evaluation of the effects of thiosulfate and other reduced sulfur species. The effect of these species on localized corrosion of C-22 needs to be resolved. They are known to extend the corrosion regions of nickel alloys.

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.

E. The Role of Fuel Cladding

Background

The UO_2 pellets in nuclear fuels are enclosed in a cladding material usually selected for its low neutron absorption and its resistance to chemical corrosion, melting and radiation damage. The most commonly used material is Zircaloy, an alloy that is approximately 98% zirconium with small amounts of tin, iron, nickel, niobium and chromium. The tubes of cladding, 600 to 900 microns thick, are fabricated by an extrusion process to eliminate seams. Fabrication and inspection techniques are employed to assure that the material is defect free. A small fraction of commercial spent nuclear fuel (less than 2%) has a stainless steel cladding and is generally considered not to be corrosion resistant under repository conditions.

A small number of the claddings of the fuel pins (0.01 to 0.05 percent during reactor operation) have failed after in-reactor irradiation, the so called "leakers" in pool storage. Cladding failure over the longer term may have a variety of causes (Rothman, 1984; Pescatore et al., 1989; Pescatore and Cowgill, 1994; Ahn et al., in press, CRWMS M&O, 1998C, Chapter 6, pages 6-19 to 6-54):

- Embrittlement due to in-reactor irradiation;
- Mechanical failure (e.g., due to handling during shipment or rock falls after disposal in the repository);
- Creep rupture;
- General or localized corrosion;
- Stress corrosion cracking;
- Chemically facilitated stress corrosion cracking due to fuel pellet and cladding interactions (Sidky, 1998);
- Delayed hydride cracking;
- Embrittlement due to hydride formation and reorientation as a function of temperature and stress field (Grigoriev and Josefsson, 1998); and
- Splitting due to volume expansion (e.g., formation of corrosion products of oxidized and altered UO_2).

TSPA-VA Approach

The TSPA-VA analysis relies heavily on the projected performance of the fuel cladding (see Vol. 3, page 4.12; Figures 3-54 and 5-29) combined with the long lifetime of the waste package canister. In the TSPA-VA analysis, juvenile (0.1%) and stainless steel cladding (assumed to fail immediately) have a combined failure rate of 1.25 percent beginning at the time of waste package failure. Long-term mechanical failure is initiated at the time of waste package failure with a rate of 0.18 percent at 100,000 years and reaches a rate of 2.62 percent at 1 million years. Failure due to long term corrosion is initiated with waste package failure with an expected value of 1.51 percent at 100,000 years and 7.75 percent at 1 million years. Thus, the fuel cladding is an important barrier which limits access of water to the UO_2. At 100,000 years no more than 3% of the cladding is estimated to have failed (vol. 3, 4-49) and not until one million years will 50% of the fuel in failed waste packages be available for dissolution (a combined result of corrosion and mechanical failure) according to the TSPA-VA. For comparison, if the cladding were completely absent, the dose rate at 10,000 years is calculated to be nearly two orders of magnitude higher than with cladding (Vol. 3, Figure 5.29). The high dose rate is primarily due to the release of ^{99}Tc at early times from the fully exposed spent fuel rods.

The analysis conservatively assumes that the juvenile failures and the stainless steel cladding completely expose the entire surface area of the fuel pellets and that this surface area is available for aqueous corrosion. In the analysis, no fuel is exposed due to creep failure and for corrosion and mechanical failure (rock falls) patches of 10 cm^2 are exposed at each penetration (the total surface area of a fuel pin is 1090 cm^2). However, the small fraction of failed claddings means that only a small fraction of the fuel is considered to have been exposed and corroded.

One of the potential means of cladding failure is by creep (although such failures do not occur as significant contributors to dose in the TSPA-VA analysis). Failure due to creep is essentially reduced to zero by maintaining the fuel pins at temperatures lower than 350° (without backfill, the maximum fuel pin temperatures reached are calculated to be between 337° and 350°C). Both creep and delayed hydride formation were considered in the TSPA-VA, but based on the analysis neither of these failure mechanisms contribute significantly to the amount of fuel available for dissolution.

The importance attributed to the role of the cladding in the TSPA-VA is further emphasized by the fact that the repository design strategy is constrained by the requirement that cladding temperatures be kept below 350°C in order to avoid hydride formation and maintain cladding integrity. Examples of such design requirements include: 1.) the absence of insulating backfill which would increase waste package temperature (the temperature may reach 380°C); 2.) limited thermal treatment of welds used to seal the end-plates to the canisters in order to remove the residual stresses from welding.

General Findings

The TSPA-VA argues (Vol. 3, 3-100 to 3-102) with substantial detail (Vol. 6, 6-19 to 6-54) that cladding failure should be minimal and that the corrosion rate of Zircaloy will be low (no more than 100 microns as compared with a cladding thickness of approximately 600 microns). Based on available data, the case for cladding credit is well made; however, substantial uncertainties remain, and this uncertainty is of particular importance because cladding plays such a dominant role in determining the outcome of the TSPA-VA analysis.

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. At temperatures less than 100°C, there are no relevant databases for irradiated Zircaloy and no information for oxidizing conditions near 100°C in dilute salt solutions (L.H. Johnson, Waste Form Degradation Expert Elicitation Meeting, January 27-28, 1998). The definition of the near-field chemistry (e.g., Cl concentration) remains critical to the analysis of corrosion mechanism and subsequent failure. 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. Thus, there is not a broad set of repository-relevant data from other national and international programs on which the Yucca Mountain Project may draw.

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. To quote from the Nuclear Waste Technical Review Board (1998),

> What needs to be determined is whether the combined interactions of corrosion products from the inner and outer walls, radiolysis, water, and elevated temperatures could produce a corrosive environment inside waste packages. Both theoretical work (e.g., using computer programs that model thermodynamic equilibrium) and experimental (laboratory) work are needed to predict the ranges of local environmental conditions that could exist inside a waste package and the probabilities of their occurrence.

The Yucca Mountain Project staff have also identified the need for a better understanding of cladding failure mechanisms (Siegmann et al., 1996):

> Additional cladding degradation processes, not considered in the current study, should be included such as stress corrosion cracking (induced primarily by iodine in the interior side of the clad, and induced by the near-field factors such as salt formation on the clad surface), long-term localized corrosion in radiolysis-induced acidic conditions, and long-term degradation under static loads which may be caused by a collapse of the internal structure (e.g., basket material). Furthermore, the degradation process(es) are likely to have synergistic effects on the other process(es); for example, stress developed by the internal pressure build-up would make the clad more vulnerable to stress corrosion cracking than the stress alone. One major obstacle to improving the current models and possibly developing new model(s) is a lack of long-term performance data. Development of testing data for such purpose is both lengthy and costly, and may not be practical in view of the time limitation for licensing.

Future Work

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.

F. Waste Form Degradation

A wide variety of waste types and compositions are candidates for disposal at the proposed Yucca Mountain Repository. Under current policy 90 percent of the waste (63,000 metric tons) will be spent commercial fuel and the remainder (7,000 metric tons) will be defense waste. Most of the defense waste will be high-level waste that has been vitrified and placed in canisters Additional waste types that are considered for disposal at Yucca Mountain include: Navy reactor fuel, DOE fuel from research reactors, and waste forms (glass, crystalline ceramic, or mixed-oxide fuel) resulting from the immobilization and disposition of excess weapons plutonium. The spent fuel assemblies and the canisters of vitrified waste will be combined into 11,000 disposal containers under the reference design. These waste types vary substantially in their chemical characteristics, radionuclide inventories, radiation fields, and thermal outputs. However, well over 95% of the total activity is associated with the commercially-generated spent nuclear fuel (CSNF); thus, the dominating source-term will be the CSNF, and the primary waste form degradation process to be modeled is the corrosion and alteration of the UO_2 in the SNF.

The waste forms (spent fuel or vitrified waste) are the first barrier to radionuclide release. Indeed, in their initial configuration in the repository, the radionuclides are entirely confined in the waste forms. To the extent that there is successful containment within the waste form, the dependence on far-field barriers (e.g., long travel times, dilution in groundwaters, or sorption on mineral surfaces) is substantially decreased. More importantly, to the extent that the waste forms are a significant and successful barrier to radionuclide release, uncertainties in the analysis of the performance of the far-field are much reduced. Thus, the Panel believes that it is important, as far as possible, to exploit the properties and behavior of the waste forms as important barriers to radionuclide release.

The principal mechanism for release of radionuclides from the waste form is by corrosion in the presence of aqueous solutions. Principal repository parameters affecting release rates are:

- The timing of the contact of the waste form with water,
- The nature (vapor, thin-films, flowing) and volume of the water,
- Water compositions (e.g., pH, Eh, chloride content); and
- Temperature.

These parameter values change with time, that is their values are sensitive to the projected or modeled future behavior of the repository. The parameters are generally characterized by a range of possible values generated by the models of repository behavior.

Principal materials property parameters affecting release rates from waste forms are:

- Thermodynamic stability of the waste forms;
- The kinetics of alteration and corrosion reactions,
- Surface area;
- Speciation of released nuclides in solution;
- The formation of alteration products and colloids; and
- The solubility limits of precipitated phases.

In general, these materials parameters may be measured by laboratory experiments or, in some cases, predicted from fundamental scientific theories or bounded by empirical results.

The key to successful and convincing modeling of waste form degradation and radionuclide release is the careful determination of materials parameters combined with a realistic definition of the corrosion environment.

Additionally, even prior to contact with water, the properties of the waste form may be affected by external parameters. Oxidation of the UO_2 can cause volume changes. Thermal events may cause devitrification of the glass. Radiation fields can change the stability of crystalline phases (e.g., increase the leach rate) or cause microstructural changes in the solid (e.g., radiolytic formation of bubbles in the waste glass) as described by Weber et al. (1997a, 1998).

In the TSPA-VA, the models used to describe waste form degradation consist of three types:

- Simplified deterministic models of waste form degradation and mobilization of radionuclides which include the most important processes expected in the repository performance;
- a "response surface" that is a fit to a set of experimental data as a function of relevant parameters generated by thermo-hydrologic models (e.g., temperature and relative humidity);

- more sophisticated process-based models used for side calculations and sensitivity analyses.

Spent Nuclear Fuel

Background

Under oxidizing conditions in the presence of water, or even moisture, the UO_2 in spent nuclear fuel is not stable. In oxic solutions, uranium has a strong tendency to exist as U^{6+} in the uranyl molecule, UO_2^{6+} Uranyl ions react with a wide variety of inorganic and organic anions to form complexes. Throughout most of the natural range of pH, U^{6+} forms strong complexes with oxygen-bearing ions like CO_3^{6+}, HCO^{3-}, SO_3^{6-}, and PO_4^{3-}, which are present in most oxidized stream and subsurface waters. At 25°C and with a typical groundwater P_{CO2} of about 10^{-2} atm., the most abundant of these are the uranyl carbonate species, which are stable down to a pH of about 5. Below pH = 5, U^{6+} is generally in the form of UO_2^{2+}. Thus in most oxic, near surface environments, uranium is easily transported in natural waters, as the U^{6+} uranyl phases have generally high solubilities (Grenthe et al., 1992).

The reaction kinetics for these alteration reactions and the formation of secondary uranyl phases are rapid. Wronkiewicz et al. (1996) estimated that UO_2 pellets in experiments (90°C in dripping water) would have been completely altered in less than 1,000 years. The alteration can occur simply due to the exposure of the UO_2 in the fuel to moisture in the unsaturated zone. The secondary phases that initially form are typically oxyhydroxides, such as schoepite. Depending on the composition of the groundwater, uranyl oxyhydroxides, silicates, and phosphates form, such as soddyite or uranophane.

Observations concerning the formation of secondary phases during experiments (Wronkiewicz et al., 1996) and at natural analogue localities (Finch and Ewing, 1992; Pearcy et al., 1994) are also supported by kinetic and thermodynamic models of UO_2 corrosion (e.g., Bruno et al., 1966) in which the final steps of the corrosion process are the precipitation and subsequent dissolution of the secondary uranium phases. Many of these secondary phases are sheet or framework structures (Burns et al., 1997, 1998) in which there is a large increase in volume as a result of the alteration. These phases may also become host phases for released radionuclides, such as Np. Thus, the paragenesis and stability of the uranyl phases are a primary consideration in the assessment of radionuclide release.

TSPA-VA Approach

In the TSPA-VA, spent fuel corrosion utilizes input on the water chemistry, spent fuel surface area and temperature to define the release of radionuclides from the UO_2 as a function of time. The release is as dissolved and transportable species (colloids). No credit is taken for the co-precipitation of radionuclides in the secondary uranyl phases. The model consists of three sequential parts:

1. An oxidation model which describes the oxidation of UO_2 to U_3O_8. This is important because of the volume increase (~30%) that accompanies the oxidation process. The

volume increase can lead to disaggregation of the fuel and an associated increase in surface area.

2. An initial rapid release of a small fraction of the radionuclide inventory that is located in the gap between the UO_2 fuel pellets and the Zircaloy cladding. The gap inventory is taken to be the volatile nuclides, such as ^{14}C, ^{135}Cs, ^{137}Cs, ^{129}I, ^{99}Tc and ^{79}Se. Generally, 2% of the inventory (Chapter 6, Table 6-27) is assumed to be available for immediate release from the gap on penetration of the cladding.

3. An equation to describe the intrinsic dissolution rate of UO_2 in spent nuclear fuel. The rate equation is a fitted response surface to a limited number of data taken from high-flow rate experiments. The dissolution is described as a function of temperature, pH, CO_3, burnup and oxygen potential. Although the rate equation finally is reduced to the classic chemical kinetic rate law, it is essentially an empirical fit of a response surface to a limited set of experimental data. As the authors of the TSPA-VA (CRWMS M&O, 1998d, Chapter 6, page 6-61) properly note,

   > However, because the model is nonlinear, extrapolation beyond the measured independent variable space could cause large prediction errors and should be used with caution.

Additionally, models are developed for metallic spent fuel, carbide spent fuel, and Navy fuel. The models for the first two are based on models used in Rechard (1995) and for the latter the source term is defined in a look-up table provided by Becket (1998). Limited data are cited in support of the use of these models.

General Findings

The spent fuel corrosion model is essentially a response-surface fitted to a limited set of experimental data (Stout and Leider, 1996, Tables 2.1.3.5-4 and 2.1.3.5-4a, CRWMS M&O, 1998c, Chapter 6, page 6-61). 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 the 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. The present approach provides only limited insight into the interpretation of even short-term laboratory experiments; thus, there is little basis for extrapolating the response-surface models beyond the experimental data sets used in the TSPA-VA analysis. 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 (e.g., Shoesmith and Sunder, 1992; Shoesmith et al., 1996; Shoesmith et al., 1998; Forsyth, 1997; Sunder et al., 1997, 1998; Serrano et al., 1998a, 1998b) or in the context of natural analogue studies (e.g., Pearcy et al., 1994; Janeczek et al., 1998). 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%) of the radioactivity is contained in the UO_2 of the spent fuel. This would, perhaps, not be so important if the dissolution rates were low; on the contrary, dissolution rates are rapid and the long-term solid-state assemblage may well be the corrosion products of the altered fuel (formed within 1,000 years after exposure to water). Although one may consider the use of a response surface as conservative (because the dissolution rates are high and the fuel matrix is converted to secondary alteration products within 1,000 years of exposure to water), the absence of a process-based model weakens the conceptual basis of other parts of the analysis (e.g., the description of the formation of secondary phases, the use of solubility-limited concentrations for radionuclides, radiolysis effects on the corrosion of UO_2, etc.).

Finally, 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-VA, these parameters have not been discussed in terms of a deterministic model which can then be used for a subsequent abstraction. There is also barely any discussion of the status of the database required to model the reaction progress and formation of the stable, radionuclide-bearing phases or the kinetics of reactions related to the spent fuel corrosion. 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.

More specific points include:

1. For other waste forms, such as ceramic spent fuel, corrosion models are extracted from rather obscure sources (Lappa, 1995) or dated sources (Reeve et al., 1989; Ringwood et al., 1988). 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. As an example, the model for the corrosion of metallic spent fuel (vol. 6, p. 6-68) is taken from Rechard (1995). The Panel found little to substantiate the use of this model in Rechard (1995). Indeed, the discussion of "Corrosion and Source Term Modeling" was less than a single page, although it did reference geochemical modeling and comparison to "several solubility experiments" conducted in J-13 well water in an Appendix E, "Scoping Calculations." Appendix E provided a brief discussion (five sentences) and comparative list of outputs for the EQ3/6 geochemical code. At no point is there any discussion of the fundamental limitations of the EQ3/6, or more importantly, the severe limitations of the database for uranyl silicates (see Chen et al., in press, for such a discussion). In the TSPA-VA, this model for the metallic fuel is further incorporated into the analysis of the DOE spent nuclear fuel by the statement, "A reasonable dissolution-rate model for this surrogate waste form is the metallic fuel model" (vol. 3, 3-98, 5-33).
2. 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 (CRWMS M&O, 1998C. Chapter 6, page 6-118) 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 SNF 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.

Future Work

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.

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;
- An evaluation of the effect of the corrosion products on the spent fuel: a.) effect of volume increase due to oxidation and alteration of UO_2, particularly on the mechanical integrity of the cladding; b.) effect on access of water to fresh corroding surfaces of the fuel (e.g., do the alteration products "plug" holes in the cladding or become a diffusion barrier to release of radionuclides);
- The effect of alpha-radiolysis on the corroding fuel surface and on the corrosion products;
- The formation of colloids on the corroding fuel surface.; and

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

Borosilicate glass

Background

Although the vitrified, defense waste will occupy a large volume (approximately 6,000 canisters of vitrified waste), this waste form will represent only 4,400 MTHM (equivalent) of the total of 70,000 MTHM of the repository capacity. The vitrified waste will account for only five percent of the total activity, and most of this activity is associated with short-lived fission products. Still, the total amount of radioactivity in the vitrified waste is substantial (approximately 10^9 curies).

It is also important to note that the alteration mechanisms of HLW glass and spent nuclear fuel are quite different (Grambow, 1998). Glass is an aperiodic, thermodynamically metastable, covalent/ionic solid whose degradation depends on ion-exchange, surface complexation and Si-saturation. In contrast, the UO_2 of spent nuclear fuel is a crystalline, redox-sensitive semiconductor whose dissolution behavior is mainly governed by redox mass balance at the oxide-solution interface. Thus, the corrosion of the spent fuel is very sensitive to radiolytic effects at the solid-liquid interface while the glass dissolution rate will be particularly sensitive to the silica-content of corroding solutions. For both waste forms, corrosion can have a major impact on solution composition (e.g., in the case of glass dissolution under static conditions the pH increases), and corrosion is accompanied by the formation of alteration phases (amorphous gels, colloids and crystalline solids). These phases may incorporate various radionuclides into their structures by precipitation, coprecipitation and sorption. Grambow (1998) has compared the kinetics of the long term rates for these two waste forms and noted that the long term rates depend critically on two different phenomena: (1) for glass, the rate is related mainly to processes associated with silica "saturation" and (2) for spent nuclear fuel, the rate is most directly related to radiolytic, oxidative dissolution. For radionuclides for which concentrations are bounded by solubility limits, both the spent nuclear fuel and the glass will be contributing (at different rates) to the radionuclide inventory of the corroding solution; thus, one must anticipate chemical interactions between these two very different waste forms which may be in the same waste package, and the assemblage of alteration products which control solubilities may depend on this interaction.

TSPA-VA Approach

The model developed for the TSPA-VA draws on several decades of work on nuclear waste glass corrosion. The defense high level waste (DHLW) dissolution rate, R, is given by:

$$R = s[k(1 - Q/K) + k_{\text{long term rate}}]$$

where s the effective surface area (m^2), k is a rate coefficient (g/m^2day) which varies as a function of temperature and pH, and Q/K is an affinity term consisting of the silica concentration in the aqueous phase divided by the solubility of silica in the aqueous phases. The $k_{long\ term}$ is the long-term rate which varies as a function of temperature, solution composition, and flow rate. Both k and $k_{long\ term}$ are determined from experimental data, and at present there is no consensus on the mechanisms described by these rate constants. The rate constants are determined by a linear regression fit to experimental data over a range of pH and temperature conditions for flow-through experiments (Knauss et al., 1990).

General Findings

The glass dissolution model used in the TSPA-VA represents a relatively straightforward, transparent approach to describing the corrosion process. The form of the representation is consistent with transition state theory, often used to describe the corrosion of glass. Extensive studies of a wide variety of synthetic and natural glass compositions have provided generally consistent results with this approach. Although the mechanisms represented by the rate constant values are not entirely understood, the rate constants may be obtained by appropriate, long-term experiments, and these values may be used to bound long-term waste form behavior (Grambow, 1998).

Much to the credit of the project, the supporting documents to the TSPA-VA (Vol. 6) clearly outline the limitations of this approach:

1. The model ignores all solution chemistry other than pH and silica concentration.
2. Absorbed species (e.g., iron from the corroding canister) are not considered although absorbed species can have an effect on the glass dissolution rate (e.g., formation of Fe- or Mg-rich phases on the surface layer of the corroding glass).
3. There is no consideration of vapor phase hydration of the glass. A breached canister may allow water vapor to reach the surface of the glass and substantial alteration may occur. The release rate of this surface in the subsequent presence of water may be higher than that of fresh glass.
4. Diffusion of radionuclides through the glass matrix and through the surface layer is not incorporated into the model.
5. The generation of colloids from the glass surface is not considered in the corrosion model.
6. No credit is taken for the retention of radionuclides in the gel layer or secondary alteration products that form during glass corrosion. This is an important issue as these alteration products may be viewed either as an efficient "sink" for rare earth elements and actinides or a source of colloids with high actinide concentrations. Greater than 90% of the actinides may be concentrated in the leached layer. Although proper evaluation of the role of the leached layer and the effects of alteration products will require more information than is presently used in the TSPA, the potential retardation of actinides in this layer may justify a more sophisticated approach that considers the role of the gel layer and alteration products.
7. There is no consideration of the potential effects of ionizing radiation on the vitrified waste (which will be mixed in the waste package with spent fuel assemblies). This issue has been raised by a recent DOE panel and should have been addressed by the TSPA-VA (Weber et al., 1997a).

Future Work

The present database used in the TSPA-VA is extremely limited and in some cases dated (Knauss et al., 1990). Much can be gained by using a wider variety of data sets, and these comparisons should be used to evaluate the uncertainty of the modeled results.

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 the extrapolated 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 rates.

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.

G. Radionuclide Mobilization

Solubility-Limited Radionuclide Concentrations

Background

Under equilibrium conditions, the concentrations of radionuclides in solution depend on the solubility products of the solid phases that contain the radionuclides. Radionuclides may form phases in which they are the dominant element, or they may occur in trace amounts incorporated into phases which are more abundant (e.g., co-precipitation). In the case of the corrosion of spent fuel, the latter will almost certainly be the secondary, uranyl phases. The solid phases that form depend on the composition of the groundwater which determines the speciation in solution, the redox conditions and temperature. Proper use of solubility limits requires a knowledge of the solid phases present and the geochemical environment (groundwater composition, Eh and temperature). Thermodynamic equilibrium is assumed; thus, kinetic barriers to precipitation or dissolution are not considered.

TSPA-VA Approach

The waste form dissolution models provide calculated upper and lower boundary values for the aqueous concentration of radionuclides in the groundwater. These values are filtered by comparison to solubility-limited values that are themselves sampled from either a distribution of solubility limits for radionuclide-bearing phases or in some cases a functional form of the solubility limit value is used. The solubility-limited value is the maximum concentration used in the analysis. The distributions for the solubility limit parameters were established for eight radionuclides (CRWMS M&O, 1998c, Chapter 3, Table 3-15, page 3-99) or in the base case calculations for 19 radionuclides (CRWMS M&O, 1998c, Chapter 6, pp. 6-80 to 6-87, Table 6-32) by expert elicitations, from previous assessments, and, in the case of Np, a reassessment of available experimental data (Sassani and Siegmann, 1998). With the exception of the distribution for Np, many of these elicitations were completed in the early 1990s. Even with the reassessment of available data, the solubility values for Np vary over three orders of magnitude, and this range does not encompass all of the experimental data. The greatest effect of the Np-solubility on dose for the base case model is in the period from 50,000 to 250,000 years when the total dose is dominated by solubility-limited release of neptunium. At longer times, the cladding degradation rate dominates the total dose rate. In the absence of cladding credit, solubility-limited release may be important over longer times. The importance of solubility-limited release of Np to the calculated dose is also increased when the seepage flux is high.

General Findings

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. At present the wide range of possible conditions in the near-field environment (which is sensitive to seepage rate, incoming gas flux and composition, extent of reactions with concrete and thermal-hydrologic interactions, to name a few) does not provide the necessary basis for describing the evolution of solution compositions over time or as a function of reaction progress.

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. In order for the project to make substantive arguments based on solubility limits, identification of the solid phases is essential. Proper identification of these phases allows one to distinguish between conceptual models (i.e., precipitation, co-precipitation and sorption). It is instructive to review the literature on experimental studies in order to establish the extent to which thermodynamic data can be used to successfully predict radionuclide concentrations in solution. A recent experimental study (Werme and Spahiu, 1998) of spent fuel dissolution under well controlled conditions demonstrated that,

   "The measured U concentrations are difficult to correlate with solubility control as calculated assuming chemical equilibrium."

   The calculated concentration using a solubility-limited model for Pu overestimated concentrations by a factor of 10, and for Np by a factor of 100. Although one may take these results to demonstrate that calculated values are "conservative", the authors of the study concluded,

   "It is our opinion that these discrepancies between the calculations and the observations of spent fuel behavior under laboratory conditions must be clarified since predicted radionuclide solubilities are used in performance assessments, and the selection of solubilities and speciation has a large effect on the outcome of a performance assessment."

3. The database for the relevant radionuclide-bearing phases is extremely limited. This remains a major impediment to the use of solubility-limited concentrations. Even if the major radionuclide-bearing phases are identified in experiments or successfully predicted by geochemical codes, there are few relevant thermodynamic data. For key elements, such as Pu and Np, the situation is even worse (Fuger, 1993):

"For the transuranium elements, especially neptunium in its quadrivalent state (and to some extent pentavalent state), and plutonium in its quadrivalent and pentavalent state, more data are absolutely required."

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. This leads to the broad ranges in the expert elicitations, but this also reduces the value or validity of the sensitivity analyses used to determine the importance of the solubility limits for individual radionuclides.

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.

Finally, the project should take advantage of the work in other national programs. SKB has recently completed a study (Bruno et al., 1997) of radionuclide solubility limits with an effort to identify the sources of the uncertainties associated with the estimated values. Principal sources of uncertainty are: 1.) variations in the water chemistry; 2.) redox conditions; 3.) temperature. They identified certain elements for which results were not much affected by these parameters (i.e., Ag, Pa, Pd, Ra, Th and Zr); however, other elements (i.e., Np, Pu, Se, Tc and U) were strongly affected by at least one of these parameters.

Neptunium Solubility:

The TSPA-VA has recently completed a reanalysis of the data for ^{237}Np solubility which lowered the range of ^{237}Np-concentrations by several orders of magnitude (Sassani and Siegmann, 1998) as compared with the values used in the TSPAs of 1993 and 1995. Previous estimates had been based on the work of Nitsche et al. (1993, 1994). In the recent reanalysis, the main points are: (1) the solubilities given by Nitsche et al. (1993, 1994) are considered to represent metastable equilibrium between the aqueous solutions and metastable Np-phase(s); (2) Np-concentrations measured in dissolution experiments are directly relevant to a system which will approach steady-state conditions from undersaturation. Thus, four sets of spent fuel dissolution tests by Wilson (1990a, 1990b), Finn et al. (1995) and Gray and Wilson (1995) were used in combination with the calculated Np-concentrations in equilibrium with NpO_2 under various conditions in order to derive additional constraints on the aqueous concentrations of Np for J-13-like fluids which initially have no dissolved Np.

As noted by the Panel in its third interim report (Whipple et al., 1998) 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). The formation of secondary phases or sorption may be the dominant process (Werme and Spahiu, 1998). 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.

Selenium

Note, the half-life of ^{79}Se is actually 1.1 million years (Jiang et al., 1997), not the 65,000 years used in the TSPA-VA (Chapter 3, Table 3-14).

Formation of Secondary Phases

Background

As discussed in the Panel's first interim report (Whipple et al., 1997), in the presence of water or water vapor, the alteration and corrosion rate of UO_2 is relatively rapid under oxidizing conditions. As modeled by the TSPA-VA (Chapter 6, Section 4.6.2.2.2) the UO_2 in the waste package will be completely converted to secondary uranyl phases within 100 to 1,000 years after waste package failure and exposure to water. Under such conditions an assemblage of uranyl oxyhydroxides, silicates, phosphates, carbonates and vanadates will form depending on groundwater compositions (Langmuir, 1978; Finch and Ewing, 1992; Wronkiewicz et al., 1992, 1996; Finn et al. 1994, 1996; Pearcy et al., 1994). It is expected (Burns et al., 1997) and has been shown experimentally (Buck et al., 1998) that certain radionuclides, such as ^{237}Np, will be incorporated into the structures of these secondary phases. Thus, the formation of these secondary, alteration phases may remove certain radionuclides from solution by coprecipitation or sorption and retard their release from the near-field environment.

TSPA-VA Approach

At present, the TSPA-VA does not take credit for this type of radionuclide retardation; however, such a possibility is under consideration and may become an feature of the TSPA-LA (CRWMS M&O, 1998d, page 5-29). The TSPA-VA does, however, include a side analysis of the effect of lowering the concentration of ^{237}Np in solution by reducing the "solubility" of neptunium by a factor of 45 to approximate the results of reactive transport modeling using the AREST-CT code. The effect on dose is considered over three time frames: ten thousand, one hundred thousand and one million years. During the ten thousand year period, there is no effect because the dose is dominated by contributions from ^{99}Tc. No effect is seen until approximately 50,000 years, and the maximum effect, at 200,000 years, is to reduce dose by a factor of 25 below the base case calculation. At that time, ^{237}Np is responsible for 99% of the calculated dose. Note, the curves for dose rate at one million years (CRWMS M&O, 1998d, Fig. 5-33) are slightly different from those presented in Chapter 6 (Fig. 6-62). The curves share the same general shape and magnitudes, but the latter curve indicates an earlier effect of secondary phase formation.

The AREST-CT code is a reactive-transport code. Two scenarios are considered: 1.) that ^{237}Np is incorporated into the uranyl phase, schoepite, in the same molecular ratios as it exists in the UO_2 of the spent fuel and is released during the subsequent dissolution of schoepite; 2.) the ^{237}Np released from schoepite is subsequently incorporated into uranyl phases, such as uranophane, Na-boltwoodite and soddyite, again in the same molecular ratios. The simulations are completed for different temperatures (30° and 70°C, or 86° and 158°C) for different cladding failure rates (1 and 11 percent). The simulated neptunium concentration at the bottom of the waste packages ranged from 10^{-9} to 10^{-6} mol/kg and an expected value of $10^{-7.5}$ was used for the sensitivity analysis described above.

General Findings

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. Although there has been considerable recent progress in the description of the structures of relevant phases (Burns et al., 1996, 1997a), the evaluation of thermodynamic parameters for these phases (Finch, 1997, Clark et al., 1998; Chen et al., in press) and the potential for these phases to incorporate radionuclides, such as ^{237}Np (Burns et al., 1997b), Pu (Burns et al., 1997c), ^{79}Se (Chen et al., in press, submitted) and ^{99}Tc (Chen et al. in preparation), the fundamental data requirements for the models used in the analysis (e.g., AREST-CT) fall far short of what is required for a definitive analysis.

Proper evaluation of the secondary phases will require:

1. A determination of the phases that form over the range of relevant conditions. Experimental work will be difficult because metastable phase assemblages may form during short-term experiments, and the phase assemblage and phase compositions will change over time. This work should be compared to phase assemblages and relative abundances as described in relevant natural analogue sites.

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. Present work (e.g., Buck et al., 1998) is preliminary. Proper work will require the synthesis of relevant phases and systematic studies to determine radionuclide solubility limits in these phases. The assumption in the sensitivity analysis that ^{237}Np will be incorporated into these phases in molar proportions to its concentration in the spent fuel are certainly not based on data nor is this to be expected. In fact, for the uranyl phases that form during the alteration of uraninite, there are indications that trace elements (and therefore radionuclide retention) may be less than expected.

3. The incorporation of radionuclides into the uranyl phases does not mean that they will be retained as long as the phase is present. The ion exchange capacity of some uranyl phases may be considerable, as they share many structural features with clays (both mineral types are composed of sheets) and ion exchange between interlayer sites and water is possible (Burns, 1998, Burns, in press). The extent of exchange will be sensitive to solution compositions.

4. An evaluation of the thermodynamic stability and/or solubilities of these phases is required. At present the thermodynamic database for these uranyl phases is limited and in some cases contradictory (Grenthe et al., 1992; Chen et al., in press).

Additionally, it has been suggested that some uranyl minerals show retrograde solubilities, that is, they become more soluble with decreasing temperature (Murphy, 1997).

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.
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. Radiolysis effects on the solution, as well as solid-state radiolysis of molecular water in hydrated uranyl phases should be considered. Ionizing radiation has an important effect on zeolites (framework aluminosilicates which contain molecular water), and the same effects may occur in the uranyl phases (Wang et al., 1998). This has been noted by the project (Chapter 6, page 6-129); however, the "caveat" implies that radiolysis effects will be analyzed. The Panel recommends that, in addition to the analysis, radiation effects be studied experimentally.

Finally, the project should take considerable care not to extend the analysis beyond the database available. The fact that the role of secondary phase formation is not yet included in the base case analysis is an example of thoughtful forbearance. However, 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. As an example, the project quotes Burns et al. (1997) to page and paragraph number in order to substantiate the fact that the substitution of Pu and Np into the secondary uranyl phases is "likely". The project fails to quote the next and last paragraph of this same paper (Burns et al., 1997):

> We emphasize that these conclusions are preliminary and confirmation will require experimental work, including structure determinations of An-substituted U^{6+} phases and chemical analyses of the alteration products formed in experiments and nature.

Colloid Formation

Background

The description of the fate of radionuclides in the Yucca Mountain Repository is essentially the description of competing geochemical processes that either retard (precipitation, co-precipitation and sorption) or enhance release and transport (the formation of molecular complexes or colloids in solution). For radionuclides with relatively low solubilities, particularly actinides, colloid formation and transport is one mechanism of providing for elevated release. Basic properties of colloids, particularly actinide-bearing colloids, have been summarized by Silva and Nitsche (1995) and Kim (1991, 1994). Depending on the nature of the colloid (e.g., size and charge) and solution composition (e.g., ionic strength, pH and temperature), colloids may either enhance or retard transport of actinides. Retardation can occur by: 1.) filtering as colloids are transported through the finely spaced fractures of the tuff; 2.) intrinsic colloids, such as Pu-oxy-hydroxides, may disassociate when they are transported from the near-field environment to the undersaturated solutions in the far-field; 3.) sorption onto rock surfaces during transport; 4.) the fact that actinides which are sorbed onto mobile geocolloids (e.g., charged surfaces of clays and iron oxides) may desorb and be reabsorbed onto rock surfaces and thus become immobile. Not only are colloids abundant in natural waters, but corrosion of materials in the drifts (e.g., concrete, iron, and the waste forms themselves) may generate colloids. Bates et al. (1992) have shown in laboratory tests of the corrosion of simulated nuclear waste glass that colloid-sized particles form in the alteration layers of the glass and contain nearly one hundred percent of the released Pu and Am. Additionally, actinides sorbed on colloids may be transported at a faster flow rate than the solute species (Savage, 1995). Thus, failure to consider colloid transport can lead to a significant underestimation of actinide transport (Ibaraki and Sudicky, 1995a).

There has been renewed interest in the potential for colloid transport due to recent results obtained at the Nevada Test Site which have been interpreted to indicate transport of Pu as colloidal material by groundwater (Kersting et al., 1999) over distances of approximately one kilometer within a period of 30 years.

Note, a Los Alamos National Laboratory summary report on colloids is being prepared but it was not yet available for review by the Panel.

TSPA-VA Approach

The TSPA-VA has focused its modeling efforts on transport of Pu via colloids. Because Pu has a low solubility and high sorption onto rock surfaces, colloid transport could have an effect on the TSPA-VA results. The model considers four types of colloids: clay, iron corrosion products, spent fuel and waste glass colloids. The attachment of Pu onto near-field and far-field colloids is expected to be reversible on the time scale of transport (hundreds to millions of years).

The TSPA-VA uses two simple models to capture the anticipated extremes in colloid behavior:

- A reversible model in which equilibrium is instantaneous and desorption is slow; and
- An irreversible model in which irreversibly attached Pu is treated as a non-sorbing tracer.

Conceptually, the approach is reasonable, but the models of colloid transport are limited by the lack of appropriate data. Colloid concentrations are estimated as a function of ionic strength. Sorption onto near-field colloids is described by a K_d in the RIP code and in the far-field by a K_c (which is a combination of a colloid concentration parameter and sorption coefficient) in the Finite Element Heat and Mass code. Because of the uncertainty in parameter estimates, the TSPA-VA uses an expected value of 10^{-7} M concentration for the Pu irreversibly sorbed onto colloids. A three order of magnitude range is attached to each side of this estimate. An important conclusion of the TSPA-VA is that plutonium transport by colloids was responsible for the peak dose in a significant number of realizations. According to the modeled results, colloid-facilitated transport is "moderately important to performance in the time period from 10,000 to 100,000 years"

(CRWMS M&O, 1998d, 6-16). These higher dose realizations could be the result of the wide range of concentrations used to describe the Pu-colloid concentrations.

General Comments

As has been properly noted by the project, the effects of colloid-facilitated transport remain one of the major sources of uncertainty in the TSPA-VA. The situation is best summarized by the project itself (CRWMS M&O, 1998d, 3-104).

> However, the necessary parameter values for modeling plutonium attachment to colloids are not available. In addition the performance assessment computer codes for modeling radionuclide transport currently cannot accommodate the complexity needed for these calculations.
>
> Specifics of colloid properties such as surface charge-size distribution and stability in expected groundwaters, and of the transport and filtration properties in the pathways within the fractured tuff, . . . are not adequately known for accurate prediction at this time.

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. As an example, ionic strength varies along the pathway (this is most difficult to estimate in the near field, but probably well known in the far field). Studies by Seaman et al. (1995) have shown that even minor changes in groundwater composition can influence surface charge and colloid generation, in their case for an iron oxide-dominated system.

Despite the conceptual utility of the models used in the TSPA-VA, the models finally will have to rely on the utilization of partition coefficients (K_d) to quantify radionuclide sorption onto colloids. There is considerable discussion in the waste management literature concerning the appropriate use of experimentally determined K_ds to represent the field-scale behavior (see, for example, the summary discussion by Langmuir, 1997). This literature is not reviewed in this report, but we simply note that the K_d values will be sensitive to parameters, e.g., pH, that are presently not included in the model (Griffin and Shimp, 1976; Bidoglio et al., 1989). The effect of pH variations has also been confirmed in field-scale studies of actinide transport (Kaplan et al., 1994). In the absence of a well defined geochemical environment the uncertainties will be large.

Finally, the sorbed radionuclides must be distributed between mobile and immobile sorption sites, and the fraction of actinide-bearing, mobile colloids is determined at the interface between the EBS and UZ models. 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.

The analysis reduces the important colloid parameters that affect Pu release to three: (1) the fraction of Pu irreversibly attached to fast moving colloids, (2) the aqueous-colloid partition coefficient (which is a combination of an assumed sorption partition coefficient and an estimated colloid concentration based on ionic strength); (3) the effective porosity in the volcanic rock of the saturated zone. Sensitivity analyses were completed on the expected dose as a function of each of these parameters (CRWMS M&O, 1998c, Chapter 6, pages 6-103 to 6-104). 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. Given the present state-of-knowledge, it would be more useful to focus the sensitivity analysis on the phenomenon itself in order to identify those physical and chemical parameters that have the greatest effect on the conceptual model of the phenomenon; in this case, colloid formation, stability and transport. A good example of such an approach is given by Ibaraki and Sudicky (1995a and 1995b).

Future Work

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. It is clear from published work (Kaplan et al., 1994) that the behavior of the actinides will differ in their ability to migrate through the system and their sorptive properties.
2. A considerable experimental database to confirm the behavior of actinides in the batch scale experiments over a range of conditions. Ideally, extrapolated results of laboratory tests should be confirmed by field-scale tests in relevant rock units.
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.
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 (Kersting et al., 1999). [?Note, please update this reference in the cited references: Nature, vol. 397, 56-59.]

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.

EBS Transport

Background

The engineered barrier system (EBS) prevents the access of water to the waste forms and is the first barrier to release of radionuclides beyond the drifts. The effectiveness of this barrier system depends on the corrosion processes and rates that lead to the breach of waste packages, the rate and volume of the water that gains access to the waste package, the mechanical and chemical integrity of the cladding, the instantaneous release of radionuclides located in the fuel gap, the waste form corrosion rates, the concentrations and means of transport of radionuclides (i.e., as molecular species or colloids) out of the waste package, transport through the steel and concrete invert below the waste package (i.e., advective and diffusive transport) and retardation due to sorption of radionuclides onto materials in the drift.

TSPA-VA Approach

As noted in the TSPA-VA, the processes in the EBS are quite complicated and many scenarios may be envisioned. This is because individual waste packages will have their own thermal and degradation histories, and the boundary conditions for each is determined by input from the models in the NFGE, the waste package and waste form degradation models, and the seepage model. Because the details of these processes were difficult to describe in the TSPA-VA, "conservative or bounding simplifications were made." These are summarized on pages 6-132 to 6-133. As with cladding failure, waste form degradation and radionuclide mobilization, EBS transport is modeled within the RIP code. The RIP code has the capability to calculate batch reactions as cells in which a cell is defined by the volume of water and mass of associated solid material. In the base case, juvenile waste package failures are assumed to cause a single patch opening on a CSNF in region 3 in the wettest environment. A single patch failure at 1,000 years was the only juvenile failure modeled.

General Findings

The modeled calculations for mobilization and transport of radionuclides through the EBS are highly stylized. As an example, the analysts considered the waste packages to be of three types (CSNF, DSNF and vitrified HLW), placed into six repository regions for 4 different environments. Each of these 72 waste package subgroups is associated with a different set of parameters that affect WP release and EBS transport. Advective and diffusive pathways are considered as connecting the waste package to the invert. Release is calculated from the waste package. The invert is divided into three cells with each cell containing water, concrete from the invert and colloids. "Placeholder K_ds" are used for sorption onto the invert where the range of values include a zero value taken to represent the possibility of flow through cracks in the invert. Although one may follow the logic of the analysis, the results cannot be reviewed without careful consideration of the actual values used in the submodels and a detailed examination of the results within and from the RIP code.

The Panel recommends that the project staff initiate a detailed, on-going review of the EBS models. Such a review should be done within the context of a similarly recommended review of the NFGE and should include the actual use and comparison of modeled results from the RIP code to modeled results from other geochemical codes and databases.

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.

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. Additionally, although the analysts have assumed, as part of the conceptual model, that the concrete materials will undergo hydrothermal degradation (CRWMS M&O, 1998c, Chapter 6, page 6-131), they have also assumed that the properties of the invert material will remain those of intact concrete (CRWMS M&O, 1998c, Chapter 6, page 6-133). 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.

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." (page 6-137)
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." (page 6-137) 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.
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." (page 6-137). 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.
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." (pages 6-137 to 6-138). Although this may be a reasonable assumption, the underlying basis is not apparent.

For the purpose of review, it is difficult to judge the cumulative effect of these assumptions on the results of the analysis.

Although in many other parts of the TSPA-VA, the sensitivities of the submodels are evaluated by a consideration of the dose estimates over time (20 kilometers from the drift), the Panel is pleased to note that, for the discussion of the behavior of mobilization through the EBS, a finer scale of analysis was used (i.e., gm/yr over time) for the transport of specific radionuclides through different pathways within the EBS (e.g., from the waste form to the invert). 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.

H. Unsaturated Zone Transport

Transport in the unsaturated zone (UZ) is concerned with migration from the repository to the water table and is controlled by the processes of advective flow, dispersion and sorption, and by the radionuclide release rates. The mechanism of transport of radionuclides that are sorbed on colloidal particles is also potentially important. Transport in the UZ shares many common issues with the Saturated Zone (SZ). In both cases, the significant issue is the determination of flow paths. The key difference is that flow in the UZ is unsaturated. This has important implications in the evaluation of the retardation of radionuclides that are subject to sorption.

Given that radionuclide movement through the UZ is advectively controlled, accurate knowledge of the flow field in the fractures and the matrix is of crucial importance for calculating travel times and concentration profiles. This is especially true for radionuclides, whose retardation, due to their sorption in the matrix of the UZ, will depend almost exclusively on the matrix flow component and the partition of flow between fractures and matrix. In the TSPA-VA abstraction, the flow fields for transport calculations are obtained based on the hydrologic model of the mountain, developed in Chapter 2 of the Technical Basis Document. A steady-state flow field is assumed and is instantly adjusted to the specific infiltration rate that corresponds to the specific climate.

As pointed out in our review of the above component on UZ flow, the estimates of hydrologic properties of the site, and particularly those affecting the fracture-matrix interaction, are subject to considerable uncertainty. Therefore, a correspondingly large uncertainty will exist for the estimation of the breakthrough curves of the radionuclides that are sorbed. Thus, depending on the value taken for the matrix-fracture reduction factor, the estimated retardation due to sorption can vary, ranging from numbers that are large to those that are negligible. Conversely, 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.

Sorption of released radionuclides will be affected by the chemistry of the environment, its alteration due to the thermal pulse, and the chemistry of water seeping through the drifts after its interaction with the canisters and the concrete liner. 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.

The stability of colloids, their retention on solid surfaces, and the transport of radionuclides on colloids are also sensitive functions of the aqueous chemical compositions, particularly of ionic strength. Their effect on the transport of radionuclides will be significant. A review of this problem has already been given in a previous subsection. The project staff has considerably improved the modeling of colloidal transport, particularly as presented in Chapter 8 of the Technical Basis Document. These efforts are moving in the right direction. 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.

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.

Other issues related to modeling, and which need to be resolved, include the effect of grid-scale hetrogeneity 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. We note the positive steps that the project staff has taken to investigate a geostatistical description of zeolitic abundance. 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.

We close by pointing out, once again, that confidence in these numerical models to simulate real processes would be considerably enhanced if they could be confirmed by laboratory and field data.

I. Saturated Zone Flow and Transport

The current treatment of saturated zone (SZ) flow and transport at Yucca Mountain is far from satisfactory. In part, this may reflect a higher level of interest and activity in UZ processes during the earlier stages of the project. This, in turn, may have resulted in less progress in SZ activities. Admittedly, the SZ encompasses a much larger volume of the mountain than the UZ. Although it does not involve the complexities of the UZ, it represents a much larger problem for site characterization, flow, and transport. 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; and
- Continuing questions regarding the adequacy of the numerical models.

The first two areas of weaknesses have forced the project staff to rely primarily on estimates of the expert panel that participated in the Saturated Zone Flow And Transport Elicitation Project (Geomatrix Consultants and TRW, 1998), for guidance on selecting values for key parameters, including dilution and retardation. As a result of comments and recommendations provided by these experts, the preliminary draft, "Saturated Zone Flow and Transport Preliminary Draft Chapter 2.9 of TSPA-VA" (CRWMS M&O, 1998a), published on February 13, 1998, has been replaced by a revised interpretation of the SZ flow and transport process. However, it is the opinion of the Panel that inherent problems remain. Additional work on this critical subject is needed. The Panel offers the following comments.

Lack of Field Data

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 Armagosa Valley, 10 km or more in length, in which no boreholes have been drilled. For this region, there is a resulting absense of data on key subjects such as: subsurface geology, water table configuration, hydraulic parameters, etc. In other words, the characterization of the SZ flow path over about one half of its 20 km length is currently not complete. 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. A more detailed discussion of the serious uncertainties resulting from this lack of data is presented in a report submitted to the U.S. Nuclear Waste Technical Review Board (Gelhar, 1998). The author of this report was one of the members of the expert Panel for the elicitation project.

The difficulty in evaluating the effects of retardation on radionuclide transport, which is needed in determining dose rate, is another inherent problem. There are two critical aspects to this problem: (1) the division of flow between the matrix and fractures in the SZ zone, and (2) the magnitude of the K_d values to be used.

According to the Expert Elicitation Panel, 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% to 20% 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 (see Langmuir in Geomatrix Consultants and TRW, 1998), 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.

Incomplete Characterization of the Site

Characterization of the site remains incomplete. 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 (as acknowledged by the project staff in Chapter 8 of the Technical Basis Document) 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.

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.

The assumed water fluxes in the SZ and UZ, their variation with different climates, and the recharge from the ground surface downgradient from the repository will also affect the description of the streamtubes. 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, as shown in Table 3.21, Volume 3, of the TSPA-VA. Indeed, instead of being constant, as required by the assumption of a constant streamtube, this ratio is shown to increase more than twofold as the climate changes from present day to super pluvial conditions.

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 MWTRB, 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.

Streamtube Approach

In response to the criticism raised by the Expert Elicitation Panel on the SZ Flow and Transport (Geomatrix Consultants and TRW, 1998), the project staff drastically revised the model of contaminant transport in the SZ in favor of a new formulation based on flow streamtubes. While the streamtube approach is better than the previous coarse-grid numerical models (200m x 200m x 20m), several issues need to be resolved.

The modeling of dispersion and dilution is treated quite empirically, using overall estimates of dilution, provided by the expert panel. 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). Development of such an approach would permit sensitivity studies to be conducted of the effects of various factors, including geostatistics, and would circumvent the necessity to rely solely on estimates from the expert Panel and/or empirical corrections. At the same time, this matter also brings up the question, also raised in the component on UZ transport, 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.

On the positive side, we note the excellent analysis, described in Chapter 8 of the Technical Basis Document, that relates the dilution factor to transverse dispersivity. The proposed convolution approach is quite useful for abstraction, assuming that processes, such as adsorption and retardation, remain in the linear regime, and the flow field is at steady state. We also note the advances in the analysis of radionuclide sorption on colloids presented in Chapter 8 of the Technical Basis Document, although these are not included in the current TSPA-VA. One of the most significant advances is that the process is now correctly treated as being dynamic, rather than irreversible.

A point should be raised regarding the fracture-matrix interaction. 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.

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 (Whipple, 1998c) 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. Even if multiple releases were to occur, the waste packages that fail could be close to one another within the repository. Such a situation could occur due to a locally aggressive corrosion environment or the fact that adjoining waste packages share a common fabrication problem.

In response to the Panel's criticism, the project 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 the 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 the exposures that would result from human intrusion and from the juvenile failure of a waste package.

J. Biosphere

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; and
- 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 of 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.

Because of the large uncertainties associated with many of the input parameters used in the biosphere analytical models, the uncertainties in the dose estimates are much larger than otherwise would have been the case. In fact, the magnitude of the uncertainties in the biosphere input parameters has led to an amplification of the impacts of the already large uncertainties associated with the analyses of the natural and engineered barrier components of the proposed repository system. Examples of the steps necessary to correct these and other deficiencies in the biosphere analyses are discussed in more detail below.

Use of Site-Specific Data

In the course of the biosphere analyses, the TSPA-VA staff conducted a major survey to characterize the diet and food sources for population groups living in the Amargosa Valley. In contrast, there was relatively little effort to obtain site-specific data on the key radionuclides that determine the dose. Such data include their adsorption and retention by local soils, their uptake by locally grown agricultural crops, their transfer from crops to other food products such as beef and chicken, and their gastrointestinal absorption factors when ingested by humans. 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. Interestingly, the data obtained in the survey of the Amargosa Valley populations are subject to considerable variation with time; in contrast, one would anticipate that data on many of the site-specific factors enumerated above to be relatively stable.

The failure to derive estimates for these parameters on the basis of knowledge of the properties of the site and region is illustrated by the following example. Although the staff recognized that the pH of the soil can significantly influence the uptake of radionuclides by various agricultural plants, they did not use this information to estimate site-specific factors for this parameter. That efforts of this type, as well as obtaining values for various parameters through measurements in the laboratory and field, are important is demonstrated by published data that show that the ratio of a given radionuclide in an agricultural plant versus that in the soil varies from 30 to 1,200, depending on the variety of the plant and the nature of the soil (DOE, 1996). It is also different, as noted by the TSPA-VA staff, for the leaves as contrasted to the root portions. Because the GENII-S code (Leigh, 1993) was used in developing the Biosphere Dose Conversion Factors, 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.

In a similar manner, the Panel believes that more attention should have been directed by the TSPA staff to the GI absorption factor for each key radionuclide. Data show (ICRP, 1996) that such factors can range from as high as 1.0 (for example, for ^{129}I) to as low as 5 x 10^{-4} (for example, for ^{237}Np) (ICRP, 1996). One apparent reason that the TSPA-VA staff did not review the values of the absorption factors for the individual radionuclides is because these factors had already been incorporated into the dose conversion factors published in Federal Guidance Reports (FGRs) No. 11 and No. 12. As such, these factors were presumed to have been properly evaluated and assessed. Even so, the Panel recommends that the TSPA staff critically review the values that were used in setting the dose conversion factors in FGRs No. 11 and No. 12. Of particular interest is how these factors vary depending on the chemical nature of the radionuclides.

Uncertainties and Conservatisms

Within Chapter 9 of the Technical Basis Document (CRWMS M&Oc,1998.), there are references to a number of conservatisms and uncertainties associated with the various assumptions underlying the dose estimates. Examples of conservatisms identified by the TSPA-VA staff include the use of the committed dose concept, and the assumption that groundwater is always withdrawn from the zone of highest radionuclide concentration and receives no treatment prior to use. In addition, 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 the dose estimates contain uncertainties. Again, however, they did not attempt to quantify them since "it would require extensive effort without providing any additional insights into the behavior of the facility" (Issues 2.04 and 2.05, page 9-26, CRWMS M&O, 1998c, Chapter 9). The amount of effort required would, of course, depend on the degree to which the uncertainties were being analyzed and the number of radionuclides being assessed. If the analyses were restricted to the key radionuclides and the key exposure pathways, the required effort might readily be manageable. Whether the process will provide insights will not be known until the task has been completed. It would also appear that a quantification of the conservatisms and uncertainties would be an important step as the TSPA staff approaches the LA stage. Useful guidance on this subject has been published by the National Council on Radiation Protection and Measurements (NCRP, 1996, NCRP, 1998). Having such information available would appear to be essential in determining whether the results of the analyses provide "reasonable assurance" that the regulatory requirements have been met.

Soil Adsorption of Radionuclides

The TSPA-VA analysis of the performance during the first 10,000 years after repository closure indicates that the estimated doses are due primarily to ^{99}Tc and ^{129}I. The doses at later times from ^{237}Np and ^{239}Pu are projected to be larger. This is due to the fact that the transport of these two radionuclides through the UZ and SZ will be delayed for extensive periods by chemical sorption and they therefore will not reach the accessible environment in significant concentrations until a considerably later point in time. 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. (Kantelo et al., 1982, Straume et al., 1996; Straume et al., 1997). 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. 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 reprocessing. Although it appears that some fraction of the deposited radionuclides may be transported to groundwater (e.g., as with cesium at the Hanford tank farm), field data suggest that radioiodine does not move unretarded through the 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. Fortunately, the staff has now recognized this problem and they are addressing it.

K. Earthquakes, Volcanism, Criticality, Human Intrusion, and Climate Change

Earthquakes

Scope and Findings

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. Based on the outcome of the analyses by the TSPA staff, the remainder of the comments of the Panel on earthquake issues will be directed to the impacts of rockfalls.

Seismic Rockfall Analysis

Background

The rockfall analysis is not (nor is it purported to be) a full TSPA analysis. Rather, it is an approximate analysis, the objective being to understand the broad features of seismic-induced-rockfall behavior and its effects in the drifts. While the analysis is quantitative, and attempts have been made to model all of the relevant phenomena, it includes many approximations and does not encompass a sufficient number of Monte Carlo realizations to explore the parameter space adequately (even given the approximate character of the models). 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.

The approximate first-look analysis in the TSPA-VA does cover all of the key issues that would need to be contained in a more thorough 10,000-year evaluation, starting by using a seismic-hazard input; then considering how the seismic motion might cause rockfalls of different sizes; and then determining how and when rockfalls might damage the waste canisters. The outcome of this analysis is an estimate of the distribution of canister-breach times and damage to the contents (the spent fuel rods) within the canister. The resulting impacts are projected to lead to increases in offsite doses as a function of time.

Evaluation

Taken at face value, the TSPA-VA analysis seems to have been reasonably well planned; it is structured appropriately, it accounts for all of the important phenomena, and it includes data sets that are, in the main, adequate for performing a first-cut analysis. The principal conclusion, that rockfall effects over the million-year time horizon seem to be an unimportant contributor to overall repository performance, appears to be reasonable and well-defended. Based on the work reported in the TSPA-VA, however, it may be more difficult to defend that same proposition with high confidence over the first 10,000-year period, considering the regulatory environment in which such a defense will take place. Specifically, it remains to be seen whether the same type of analysis, applied to the first 10,000-year period, will provide a sufficiently adequate picture of the importance of seismic-induced rockfall for the U.S. Nuclear Regulatory Commission staff to judge, should the project reach the LA stage, whether the proposed repository complies with their regulations. The regulatory-review process likely to exist will probably require a much higher level of technical rigor than is evident in the current analysis and its documentation.

The analysis elements are in hand, but they are approximate, omitting some phenomena whose absence needs either to be convincingly defended or to be included in a more elaborate model (see examples below). In addition, some of the data sets may need to be refined, and the models may need to be developed at a finer level of detail than the admittedly coarse-grained approach that was used at the TSPA-VA stage.

What remains to be seen is whether, when the 10,000-year time period is explored more carefully, the bottom-line "results" produce changes to the estimated offsite doses that are so small that little more will be required. If so, fine; if not, this area may need much more work before a defensible analysis for the LA will be in hand. Based on the limited analysis here, the effect on doses seems to be minor in the first-10,000-year period, and both the analysis and the supporting arguments appear reasonable.

Specific Comments

In terms of the rockfall analysis, the Panel has made the following observations and/or offers the following comments:

1. For the seismic-hazard input, the TSPA-VA staff has relied on the Yucca Mountain project. Probabilistic Seismic Hazard Analysis (PSHA) and appears to have done so in an appropriate manner. (The Panel, however, has not peer-reviewed the PSHA itself.) Interpreting how to use the PSHA to obtain ground-motion and ground-displacement levels underground requires skill, but it seems to have been done appropriately (albeit, approximately.)

2. A model has been developed for estimating the decrease in canister wall thickness as a function of time. Using this model, estimates have been made, for each wall thickness, of the minimum rock size that could damage the canister either by initiating a crack or by creating a crack through the canister wall. These estimates have been combined with the distribution of earthquake-induced rock sizes, based on observed joint frequencies in the existing Exploratory Studies Facility drift. This part of the analysis uses a technique, called the Rock Quality Indicator approach, to characterize rock quality. This technique seems reasonable and useful. The overall analysis appears acceptable, although the procedure for binning some of the parameter intervals may be too coarse, and could easily be refined. A more refined analysis may be needed for the LA stage.
3. The canister-damage model, while approximate, seems adequate for the purposes at hand for the TSPA-VA. However, if seismic-induced-rockfall damage to a few canisters in the initial 10,000-year period proves to be a crucial contributor to overall offsite doses during that period, then this model will need to be refined. This could easily be the case. If the canisters can be shown to be resistant to ordinary corrosion damage for the initial 10,000 years (that is to say, water intrusion proves not to be an important source of canister failure), and if the drifts are not backfilled, then seismic-rockfall-induced damage could be an important, in fact, a dominant, mechanism for canister failure.
4. In terms of the rockfall phenomena themselves, the approach used by the TSPA-VA staff is a reasonable first effort, and the projected impacts appear to be reasonable. For the LA phase, however, it seems likely that, either the simulation approach needs to be refined to account more appropriately for asymmetrical rockfalls and multi-coherent-rockfall patterns, or the omission of the potential effects of these failure patterns will need to be defended more convincingly.
5. The manner in which the time-of-breach information is matched to the WAPDEG-RIP interface may also need to be refined.

Summary

1. Estimates based on the rockfall analysis are that the resulting increases in the offsite annual doses will be small until well past 10,000 years. These results appear to be reasonable. Perhaps this type of scoping analysis will be sufficient to permit this issue to be resolved during the regulatory review of the LA. If not, various refinements (mentioned in passing above) will be necessary. 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.
2. From the perspective of the Panel, it appears likely that all of the refinements necessary to develop a more robust rockfall analysis for the 10,000-year regulatory period are within the technical reach of the TSPA staff; in most cases, these refinements are already "almost" in hand. Thus, while more could have been done at the TSPA-VA stage, the "more" is not too far beyond what has already been accomplished.

Volcanism

Scope

For the analysis of the impacts of volcanism, the TSPA staff began by developing an elaborate set of mutually-exclusive potential igneous-activity-volcanism scenarios. Three of these were then selected for detailed analysis. These were (i) a direct-release scenario in which a volcanic vent coming up through the repository carries waste material to the surface where it becomes airborne and rises to a considerable height (in this case, the airborne-respirable exposure pathway will dominate exposures); (ii) an enhanced-release scenario in which the magma never reach nor carry material to the surface but do reach the waste packages (where the magma compromise canister integrity and thus modify the base case scenario of radioactive waste materials being transported downward through the UZ to the SZ and ultimately to offsite receptors); and (iii) a scenario involving indirect effects on groundwater as a result of igneous activity having disturbed the base case UZ and/or SZ flow and transport.

The stated rationale for these selections is that they represent quite different classes of phenomena, and also are thought to bracket all of the other potential scenarios, that is to say, the TSPA staff concluded that, if the effects of these scenarios are found to be minor, the argument can likely be made that the entire range of potential igneous activity will produce only minor effects on peak annual doses. On the basis of our review, the Panel concludes that the scenario-selection process was reasonable.

A basic consideration in the analysis is the overall probability per year of an igneous event. Based on the DOE Probabilistic Volcanic Hazard Analysis (PVHA), the mean probability for such an event is in the range of slightly in excess of 10^{-8}/year, that is, slightly in excess of 10^{-4} in 10,000 years. On the basis of its letter report to DOE (Stablein, 1998.), it appears that the USNRC staff has tentatively concluded that the rate is about two orders of magnitude higher, or at least the USNRC staff believes such a rate cannot be excluded and therefore ought to be used in the analyses. As best the Panel can determine, extensive discussions between the staffs of the two agencies over the past two years have not resolved this difference. This, in turn, leaves unresolved whether the entire class of igneous events can or cannot be dismissed on probability grounds. Unfortunately, the Panel is in no position to provide a technical review of the issues pertaining to the rate of igneous activity. However, as noted below in the discussion of consequences, this is not the only difference.

This direct-release scenario has been the subject of a major amount of work by the TSPA-VA staff. As a consequence, many of the related phenomena have been explored in far more depth than those of any of the other disruptive events (earthquakes, human intrusion, criticality) bèing considered. The modeling assumptions used by the TSPA-VA staff in analyzing this scenario seem reasonable (specifically, although they are stylized, there is not constitute undue conservatism). In the scenario studied, an igneous dike emerging below the repository is assumed to interact with a few canisters in each drift and, at one location along the dike, a vent develops through which radioactive materials can be transported to the surface and into the air. The entrainment-of-canister-waste aspect and the transport-of-waste-to-the-surface aspect both seem to have been modeled using plausible approaches, accounting acceptably for magma densities and velocities, canister and waste properties, and volcanic-vertical-transport phenomena. Although the TSPA-VA staff used a standard code to perform these parts of their analysis, the Panel has not be able to review the airborne-transport-and-dose aspect (once the radioactive material has become airborne) in the form in which it is currently documented. Of note is the fact that the resulting peak doses to receptors downwind were estimated to be in the range of one hundred to a few hundred millirem, dominated by direct inhalation during the (very rare, low-probability) event, were it to occur.

Taking both the probability and the consequences of this particular scenario into account, the analysis presented by the TSPA-VA staff appears to support a conclusion that this particular exposure pathway is not an important contributor to dose rates to offsite population groups. However, the USNRC staff, in its letter report (Stablein, 1998), has described the results of its own analysis of the direct-release scenario. Although the USNRC analysis also appears entirely reasonable on its face, accounting for the same phenomena in ways apparently similar to the approach of the TSPA-VA staff, the USNRC peak dose rate estimates are two to three, and perhaps as much as four, orders of magnitude higher. In addition, the USNRC staff has apparently concluded that the likelihood of the initiating events could be as high as 10^{-2} in 10,000 years (10^{-6} per year). This estimate, combined with their higher dose rate findings, would appear if true to make the proposed repository unacceptable. The Panel was not able to review the USNRC analysis in detail. Although a resolution of these differences has not yet occurred, it appears that the difference in the TSPA-VA and DOE staff estimates may be in the interpretation and values of the parameters assigned to the airborne-ash-to-receptor pathway; at this point, however, this is yet to be confirmed.

According to the TSPA-VA analysis, neither of the other two scenarios (the enhanced-release scenario and the indirect-effects scenario) seems to be important. Specifically, the TSPA-VA staff found that neither of these scenarios produced an estimated peak dose rate even close to being of concern. The analyses by the USNRC staff do not challenge this broad finding, and they also seem reasonable to us.

Summary

The TSPA-VA volcanism analysis represents an enormous body of work on several subjects. These include how magma behave in the natural piping and in the drifts; how the volcanic materials can engulf canisters, or transport their contents to the surface; and how these materials, in turn, might become dispersed into the air. It builds on the PVHA hazard study that was also an enormous undertaking. The detail in the TSPA-VA is staggering in its complexity, far more than for any other of the disruptive events. 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.

Criticality

Regulatory Background

The new USNRC draft regulation, 10 CFR 63, treats postclosure criticality as just another process to be examined, along with all other phenomena, in evaluating the potential impacts of the proposed repository. This is a major clarification, in that an ambiguity in the earlier USNRC regulations (Part 60) had led some members of the DOE staff to conclude that potential criticality occurrences would need to be precluded throughout the post-closure period. Fortunately, the TSPA-VA staff has treated the criticality issue in the spirit of the newly proposed USNRC regulations.

Scope

The TSPA-VA staff has considered the potential occurrences of criticality in three different regions: within the canister, outside the canister but within the engineered system (the drift), and well outside the engineered system, namely, in the host rock. This is an appropriate starting point.

The TSPA-VA staff began their analysis with an attempt to delineate all of the many different potential ways through which criticality can arise. This was accomplished by developing a large decision-tree structure that differentiates among dozens of logically different scenarios. The staff then worked with this decision-tree structure to select a small number of scenarios for actual analysis. They argued that the scenarios selected represented a conservative set in the sense that the impacts of potential occurrences of criticality in the selected set would bound the impacts of all the others. The bounding criterion that they used was based either on the probability that a criticality may occur, or its potential consequences, or both. Although the accompanying arguments are not rigorous, they seem quite reasonable. Whether the arguments can survive a regulatory review remains to be ascertained -- perhaps further work will be needed, although if the results of the analysis done here (showing that criticality is unlikely to be important, and with orders-of-magnitude of margin) stand up to review, then perhaps arguments about scenario-selection will not be so important.

Conclusions

A key overall TSPA-VA conclusion is that only in-canister criticality is of even potential concern. Potential out-of-canister criticality events, either in the drift or outside the drift in the host rock, are dispensed with, using mainly probability arguments. Although they are not rigorously developed, these arguments seem reasonable to the Panel. A second principal conclusion, based on a detailed analysis of one specific scenario, is that potential in-canister criticality scenarios (i) are unlikely, and (ii) would produce only modest increases in doses offsite, were they to occur.

In terms of in-canister scenarios, the analysis was limited to evaluations of the potential occurrence of criticality in a spent-fuel canister; analyses were not performed for canisters containing defense waste or glass. The single in-canister scenario that was chosen for analysis involved a commercial-spent-fuel canister that turns into a "bathtub" when a hole develops in the top, via corrosion, through which water enters, while the remainder of the canister remains sufficiently intact to hold the water. (A "flow-through" scenario was also considered, in which a bathtub was assumed not to be formed, but its probability for occurrence was judged to be much lower.) A process is then assumed to occur within the "bathtub" that physically removes a sufficient amount of neutron-absorber material from the vicinity of the uranium/plutonium fuel, while leaving it in a critical configuration and surrounded by enough water moderator, for a critical event to occur. This removal is assumed to occur through either dissolution or physical flushing.

The TSPA-VA staff has developed both a probability for this scenario to occur and the associated consequences in terms of fission products releases. The analysis was performed for 15,000 years, and was based on an evaluation of a canister consisting of the older stainless-steel alloy (not the CAM/CRM design used in the rest of the TSPA-VA analysis). The analysts argued that for times earlier than about 15,000 years, the chances of a canister developing a bathtub configuration are much reduced, because of the integrity of the canister outer shell. (This part of the analysis will need to be revisited at the LA stage after the final canister design has been selected. The final canister will almost certainly be different from that evaluated here.) Also, it is argued that commercial spent fuel is most reactive at about the 15,000-year time period. The postulated criticality event was analyzed for criticality durations lasting for 1,000, 5,000, and 10,000 years, always beginning 15,000 years hence.

On the probability side, the overall conclusion is that the probability-per-canister of developing an in-canister criticality event, for the assumed scenario, is low, less than 10^{-8} per year. This probability is so low because each of the postulated contributing factors is itself of low-probability. These factors include the likelihoods of a bathtub configuration, of fuel/absorber separation, and of a critical configuration occurring with sufficient moderator present, combined with the probability that a criticality, once begun, can be sustained. The largest contributor to the low probability is the difficulty of developing a reasonable and physically possible sequence of events that would separate the neutron absorber from the fissionable fuel. (Notice, however, that the analysts do not claim that an in-canister criticality is "impossible". They acknowledge that it is "possible".)

On the consequences side, a single-canister criticality event was found to add several percent, at most, to the fission-product inventory already there, were the criticality to occur about 15,000 years hence. This is a key finding, indeed perhaps the key finding of this analysis.

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. A "juvenile canister failure" is a canister that has lost its physical integrity early in the repository lifetime, perhaps even by the time the repository would be closed; usually the cause of such a postulated failure is thought to be a possible manufacturing error or error during installation. Such juvenile failures are assumed and evaluated in the base case analysis, but not for 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.

Summary

The single in-canister criticality analysis that was performed seems to be quite robust. Several conservatisms are introduced both for the sake of ensuring that the outcome of the analysis will be acceptable, and for the sake of making the problem analyzable and transparent. Altogether, incorporation of these conservatisms seems to provide a "result" indicating that in-canister criticality is unlikely to be an issue for the proposed repository. However, the TSPA-VA analysis is still screening in character, and includes several aspects that will need to be firmed up to withstand a detailed licensing review. 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. Nonetheless, it appears that all of the tools necessary to achieve these needs during the possible LA phase are available.

Human Intrusion

Scope

In the human-intrusion analysis, the TSPA-VA staff has examined one stylized scenario that has been selected for purposes of a "trial run." This approach has been adopted because, as of now, there is no regulatory guidance on what to analyze. Ultimately, the USNRC regulations (in concert with the USEPA standards) will probably specify one or more inadvertent-human-intrusion scenarios that must be considered. At the time the TSPA-VA staff was developing its current analysis, neither the USEPA standards nor the USNRC regulations were available. (The draft USNRC regulations, 10 CFR 63, were released for public comment after the TSPA-VA work reviewed here had been completed.)

Stylized Scenario

The stylized scenario that was analyzed in the TSPA-VA is based on the assumption that an inadvertent intruder, in seeking to obtain groundwater, drills a single borehole at the repository site. This event is assumed to occur at a point in time 10,000 years into the future, but using today's drilling technology. The analysts further assumed that the intruder proceeds to drill right through a canister without noticing that the repository has been intersected, continues to drill all the way down to the saturated-zone (SZ) horizon, and then abandons the hole. In the process, everything that the drill bit has struck and chewed up is assumed to have been deposited at the bottom of the hole (at the top of the SZ) by the drill bit, or perhaps it all falls down the hole after the drill bit has been removed. Either way, the waste is assumed to be extensively pulverized by the time it reaches the SZ. The radioactive material present at the top of the SZ is then assumed to be available for transport downgradient with the groundwater to the accessible environment. The objective of this analysis is to determine whether a single such inadvertent borehole, at 10,000 years, will add significantly to the offsite dose rate profile estimated in the base case. There is no probability calculation; the single-borehole case is an add-on scenario assumed to occur without regard for its probability.

For purposes of the TSPA-VA analysis, it was assumed that the intrusion would occur at 10,000 years because, for the current TSPA-VA canister design that incorporates both a thick steel CAM outer cover and a thinner CRM inner layer, it was determined that until about 10,000 years hence (when substantial degradation of the outer steel CAM is projected to occur), a driller using today's technology would not be able to penetrate the canister wall.

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.

Another observation on the part of the Panel is that, if the USNRC regulations ultimately promulgated limit the period of regulatory concern to 10,000 years, then in all probability the human-intrusion scenario that will be specified needs to be assumed to occur much earlier -- for example, perhaps at 1,000 or 2,500 or 5,000 years. If the ultimate canister design is similar in certain physical/strength/thickness properties to that used in conducting the analyses for the TSPA-VA, then perhaps it can be demonstrated that with today's technology the canister would not be penetrated. (Of course, it is also possible that the USEPA and/or the USNRC will specify that the drill bit nevertheless does what has been assumed for purposes of the scenario.) Absent the existence of either the standards or the regulations, the Panel in the conduct of its review has concentrated on methodological insights. In light of the fact that the TSPA staff is continuing to evaluate possible canister designs as they progress toward the possible LA phase, the Panel has concluded that no useful insights of a quantitative nature about the robustness of the proposed repository in terms of its resistance to human intrusion have been generated by the analyses to date. Indeed, even qualitative repository-performance insights are suspect, but methodological insights are of value.

Evaluation of Methodology

The analysis of the impacts of human intrusion is reasonably straightforward, if the proposed scenario is accepted in full. The only decisions the analyst has to make are to determine (i) how large a hole will be bored through the canister, and (ii) the fate of the material deposited in the SZ as it makes its way downgradient with the groundwater toward the postulated human receptors in the Amargosa Valley.

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. 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.

Climate Change

Predictions of climate change are notoriously difficult to make and, of course, impossible to confirm. Based on the existing state-of-knowledge, however, climate-change experts believe that the current interglacial period, which has lasted for the past several thousand years, will inevitably end (Rod suggests that a reference be cited for this statement). Exactly when this will happen is not known, but the historical record over the last two-million-years-plus appears to be most consistent with a projection that glaciation will return several thousand years hence. But it could happen sooner. It is considered unlikely to be delayed, however, to the 20,000-plus-years-hence period. For its onset to be delayed that far into the future would be inconsistent with the current interpretation of the historical record. The projected glaciation would probably, as in earlier such periods, cover much of northern North America, but it would not reach as far south as Yucca Mountain, where the principal effect would be substantial cooling and increased precipitation.

The TSPA-VA staff assumed that the glacial conditions will return sometime between 1,000 and 10,000 years hence. Analyses were performed for different dates-of-return. The Panel has no reason to question the approach used for incorporating the effects of climate changes into the rest of the analyses. In fact, the results of these analyses provide important insights. For example, as the current interglacial ("dry") period yields to the wetter conditions during the glacial period (which in projected to last for many tens of thousands of years), the infiltration rate through Yucca Mountain is projected to increase from the estimated present-day annual value of 7 mm to a long-term average of about 40 mm. Estimates show that this change will have a pronounced effect on repository performance thereafter, because such a large increase in the amount of water percolating through the mountain would affect many key phenomena, all of which must be accounted for differently than in the case where current interglacial conditions prevail.

The four performance factors most affected appear to be the fraction of waste packages that experience liquid drips, the transport time for water through the unsaturated zone, and its subsequent transport time and dilution in the saturated zone. The number of waste packages experiencing drips is highly sensitive to the infiltration rate. The TSPA-VA staff has estimated that this fraction will increase from about 1% under current climatic conditions to about 30% after the interglacial period ends. (This is important because the current model projects that packages not experiencing drips would generally last 100,000 years or more before failure.)

As in the case of the return times for glacial conditions, the Panel believes that the approach taken by the TSPA-VA staff is reasonable. Furthermore, the Panel believes that the staff has sufficient modeling capability and data to perform whatever analyses of the effects of climate change will be needed for the LA stage (driven by whatever future climate conditions are assumed to occur.) In this regard, it seems clear to the Panel that it would be best for both DOE and the regulatory process if either the USEPA or the

USNRC were to specify, by rulemaking, the assumptions that would be considered appropriate regarding future climatic conditions, Provision of such guidance would help avoid, during the anticipated licensing process, contentious arguments that will inevitably develop. If such a regulatory position does not emerge, then the TSPA staff will perforce need to take a position and proceed. If this proves to be the case, it will be difficult to defend whatever assumptions are made, because the issue is unknowable.

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.

Appendix A: Specific Comments on Sub-System Models of the NFGE

The detailed conceptual models for the NFGE (CRWMS M&O, 1998c, Chapter 4, Section 4.2) describe most of the possible processes and factors that might affect incoming gas and water compositions; however, there are many parameters and processes that are described in the conceptual models which probably cannot be modeled quantitatively. Moreover, many of the key physical and chemical parameters are not known. Thus, considerable judgment must be used in the conceptualization and implementation of process-based and abstracted models of NFGE behavior. The following specific comments focus mainly on the process-level models in order to qualitatively assess sources of conceptual and parameter uncertainty.

Models of Incoming Gas, Water and Colloids

Gas

The model for in-coming gas combines a model for "air" composition in the mountain, essentially atmospheric, with the results of thermal-hydrology calculations of gas flux (a mixture of steam and air). The thermal-hydrologic results are meant to describe the effects of boiling and gas flow on the mixture of air and steam, but the analysis does not include the effects of water-rock chemical interactions.

The flux and air-mass fraction are defined by the mountain-scale thermal-hydrology (TH) model in the TSPA-VA model. This two dimensional thermal-hydrologic calculation for a cross section at about the center of the repository block (a cross-section at N233,400) provides both the air-mass fraction and the gas flux through the drift as functions of time. The air-mass-fraction variations and the changes in air fluxes delineate periods for which the gas composition is considered to be constant. These constant periods are modeled as step functions of the more continuous thermohydrologic results. Variations are modeled in more detail for the early "boiling regime" than for the later periods that represent below boiling conditions, the "cooling regime".

The incoming air is regarded as a mixture of N_2, O_2 and CO_2. These values are not calculated, but based essentially on the relative volume percentages of these components in the atmosphere. That is, the relative value of oxygen and nitrogen are about 20 and 80 volume percent, respectively, throughout all periods, except when the partial pressure of the N_2 is adjusted to 70 volume percent in the first 200 years to offset the increased CO_2-concentration in this initial period. Although the volume of CO_2 is generally low as compared with O_2 and N_2, CO_2 directly affects the pH of water and strongly affects the potential transport of actinides (e.g., as carbonate complexes). The ambient value of the CO_2 gas fraction in the air is taken as 1000 ppmv (parts-per-million by volume), and a value of 100,000 ppmv (10 volume percent) is designated for the first 200 years to reflect enhanced CO_2 in the gas due to reaction with heated calcite and silica to form calcium-silicates, degassing of CO_2 from heated water, or release of carbon dioxide from the water-mineral reactions.

As presented, the incoming-gas model is essentially based on the argument that under ambient conditions, the air composition may be represented by the pore gas composition in the unsaturated zone (UZ) and that measurements have demonstrated that the UZ ambient pore gas composition is similar to that of atmospheric air except that the CO_2 gas concentrations are elevated to values of 350 - 1,000 ppmv. This is entirely based on the assumption that thermal-chemical effects on the surrounding rock and concrete will be minimal. The assumption that the concentration of CO_2 in the air is 1000 ppmv, although logical, is arbitrary. The thermal effects on air flow and composition could be substantial, and there is no compelling argument that these variations are adequately captured by the assumption that the CO_2 concentration is 10 volume percent during the first 200 years. Thus, the conceptual and parametric uncertainties associated with gas flow and composition are large; this is critical, as the CO_2-concentrations have important affects on solution composition and actinide mobilities.

Water

The NFGE component of the TSPA-VA obtains the incoming-water flux from the mountain-scale unsaturated zone flow model in the TSPA-VA. This is done without consideration of the fully-coupled effects of the thermal pulse on the mechanical, hydrologic and chemical properties of the repository rocks.

The 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.

Chapter 4 of the TSPA-VA does not provide detailed information about the constraints that were used to determine the incoming-water flux. Instead, the model implementation focuses on the discussion of incoming-water composition.

The model implementation of incoming-water composition is based on the process-level calculations using the EQ3/6 geochemical code. In the process-level calculations, initial concentrations for the main element components are taken from the average composition of J-13 groundwater. The water composition was considered to be changed by reactions driven by heating of the system to various temperatures. In the heating process, the water is considered to react with minerals in the tuff and fracture linings, and this water equilibrates with the gas phase at various temperatures. Because boiling is expected to occur in the early period due to the repository heating followed by a cooling repository, two temperature-regimes are defined: a boiling regime and a cooling regime. There are differences in the model implementations for the two temperature regimes.

Cooling regime implementation: This period corresponds to the abstracted periods D, E and F with abstracted temperatures of 70° C, 50° C and 30° C, respectively. For each of these periods, a mass transfer model was not used to simulate the composition change in the water due to heating from the ambient to respective temperatures. Instead, a single model calculation was performed using the EQ3NR code. In these calculations, the equilibrium oxidation potential was constrained by the oxygen fugacity, and the total dissolved carbon dioxide was set to equilibrium with the CO_2 fugacity. Fixed concentrations were designated for Na^+, K^+, Sr^{2+}, Li^+, $B(OH)_{2(aq)}$, Cl^-, NO_3^-, SO_4^{2-}, F^- and

HPO_4^-. These constituents represent the total masses of these components that may be composed of a number of different species in solution. Constraints for the concentrations of other components are as follows:

Si^{4+}:	α-cristobalite
Al^{3+}:	calcium-montmorillonite
Fe^{2+}:	calcium-nontronite
Mg^{2+}:	calcium-saponite
Ca^{2+}:	calcite
pH:	charge balance

Because the fugacity values of O_2 and CO_2, which determine the oxidation potential and the pH of the in-coming water, result from the incoming-gas model, uncertainties from the incoming-gas model results add an important source of uncertainty to the modeled in-coming water concentrations. The scientific basis for the use of fixed major element concentrations, which were not considered to be functions of temperature for Na^+, K^+, Sr^{2+}, Li^+, $B(OH)_{2(aq)}$, Cl^-, NO_3^-, SO_4^{2-}, F^- and HPO_4^- is not clear.

Even for fixed concentrations, the phase stability relations may vary considerably as a function of temperature. As an example, Fig. ? represents the mineral stability relations in the system SiO_2-Al_2O_3-Na_2O-K_2O-H_2O (actual units are not given on the axes, as these will shift as a function of temperature). The minerals indicated in Figure A-1 are frequently found in geothermal systems (Browne, 1978). In almost all the ancient and active hydrothermal systems that are developed in acidic volcanic and intrusive host rocks, albite (or Ab-rich plagioclase) and potassium feldspars are altered to form clays, such as sericite, Na-montmorillonite or, under more acidic conditions caused by steam heated groundwater, kaolinite. Hydrothermal potassium feldspar and low-albite are rarely found, but are always associate with sericite. These simple observations challenge the conceptual model in which "the water should be undersaturated with unstable feldspars (e.g., sanidine, plagioclase), and supersaturated with respect to stable feldspars (e.g., albite, K-feldspar, maximum microcline) (CRWMS M&O, 1998c, Chapter 4, page 4-47 to 4-48). Such over simplifications in such a highly complex geochemical system probably do not give useful results. 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.

Boiling regime implementation: In the boiling regime, the water is considered to have been heated to 95°C, at which temperature 90 percent of the water is evaporated with mineral phases precipitating as the solution becomes more concentrated. The model implementation includes: (1) equilibration of the initial J-13 water composition at 95° C and the abstracted gas fugacities of the three boiling regime periods; (2) boiling until 90 percent of the water evaporated.

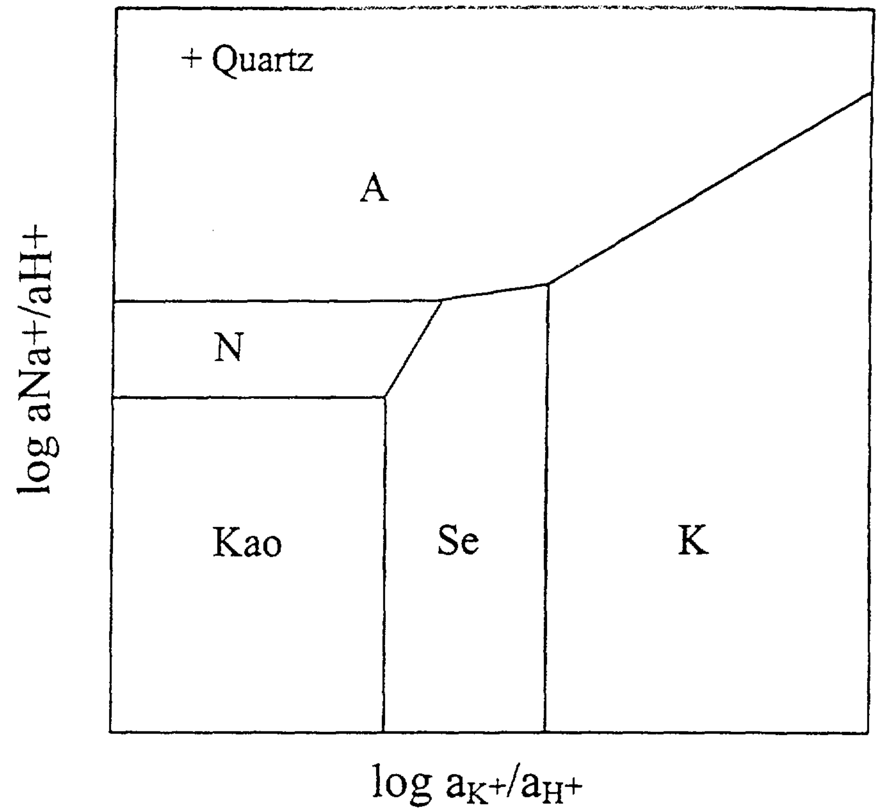

Figure A-1. Schematic stability relations among the minerals found in typical hydrothermal systems. Kao: kaolinite, Ser: sericite, NM: Na-montmorillonite, Ab: albite, Kf: K-feldspar (after Browne, 1978).

The first step of the model implementation was done by calculation using EQ3NR with the same constraints as used in cooling regime implementation. This provides an initial starting point for performing the reaction mass-transfer calculations of boiling using the EQ6 code. The sources of uncertainties in the model implementation of the cooling regime also apply to the first step in the calculation with EQ3NR. It is important to note that these calculations involve the suppression of formation of certain phases (e.g., quartz, tridymite and talc) whose formation should be hindered by kinetics. Such decisions are commonly made by analysts, but require careful justification based on experimental data and observations of natural systems. 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.

Colloids

The incoming-colloids are considered to be the natural colloids (i.e., excluding colloids formed in the drift due to the degradation and corrosion of waste-packages and waste forms) that can become mobile hosts for sorbed radionuclides. 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 (CRWMS M&O, 1998c, Chapter 4, Fig. 4-31). 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. Additionally, the site-specific measurements and the global compilations may not be relevant to a repository that has experienced an extended thermal period. 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).

Modeling of In-Drift Gas

The compositions of the in-drift gas were calculated based on the cumulative fluxes of each constituent gas as determined by the incoming-gas model implementation. Thus, the uncertainties in the incoming-gas implementation will propagate through to the calculated in-drift gas composition. The in-drift gas composition will be substantially affected by in-drift chemical reactions. The relevant calculations were not made as part of the base case presentation; however, side calculations were made as part of the sensitivity analysis in order to bound the reaction effects on in-drift gas fugacities. 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.

Other sources of uncertainty in the in-drift gas model implementation include:

1. 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.
2. According to our understanding of the in-drift gas model implementation, the total pressure of the in-drift gas is assumed to be 1 atm, and the partial pressure of each constituent gas was calculated based on its cumulative molar fraction in the drift (the partial pressure of steam is presumably set to the saturated partial pressure of water, but this is not clear). However, 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.

Modeling of In-Drift Water/Solid Chemistry

The in-drift water/solid chemistry model is used to describe the mass-transfer reactions pertinent to the interactions among gas, water, solid phases, colloids and microbial activity. The in-drift water is considered to be in equilibrium with the in-drift gas. The interactions between the incoming-water, the in-drift gas and the water-solids chemistry (e.g., precipitates/salts, concrete, steel corrosion products and spent fuel/secondary products) are summarized in Fig. 4-12 (CRWMS M&O, 1998c, Chapter 4).

Base case: The in-drift water drips directly onto the waste package and equilibrates with the corrosion product without reaction with concrete. This conceptual model is based on the assumption that the concrete liner will collapse in a few thousand years. The EQ3NR code was used to simulate the equilibration of the incoming water composition with goethite, FeO(OH), which represents the corrosion product of the waste package. The primary effect on the water chemistry from this reaction is on the dissolved iron content.

Water/concrete reaction: These reactions are evaluated by a sensitivity analysis in order to bound their influence on in-drift water chemistry. Concrete adjacent to the waste package provides concrete-modified fluid through diffusive migration of alkaline components into the waste package. This fluid can affect the rates of steel waste package and waste form corrosion.

A reaction path calculation with EQ3/6 code was used to model the mass-transfer of water/concrete reactions. Concrete is composed of cement, aggregate and iron fiber. The mineral assemblage for the cement is considered to be ettringite, Ca-silicate hydrate, brucite, Fe-hydrogarnet, Al-hydrogarnet and portlandite, which represents a "young" cement mineral assemblage as proposed by Hardin et al. (1998, in Section 7.1.2.1). Aggregate is represented by the mineral assemblage alkali feldspar, α-cristobalite and quartz. 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.
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.
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.
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.

Spent fuel corrosion and the formation of precipitates/salts: These effects are not modeled in the base case, but rather are handled in a sensitivity analysis particularly to evaluate the behavior and mobility of Np.

The water/spent fuel reaction is divided into two stages: Stage 1 describes the alteration of the UO_2 to secondary alteration phases; Stage 2 the reaction of water with secondary phases formed during the first stage. The modeled result indicates that CSNF within a waste package will be totally altered to secondary uranyl phases in a short period of time (100 to 1,000 years) once the waste package fails and the spent fuel is exposed to water.

The reactive-transport code AREST-CT was used to evaluate the effect of spent-fuel alteration on the bulk fluid composition. This code considers both equilibrium and kinetically controlled reactions between water and spent fuel. The spent fuel is represented as a one-dimensional porous medium with various specific surface areas. Parameters needed for the calculation include dissolution rates of reactant phases, porosity of the spent fuel, pore-water velocity, equilibrium constants and precipitation kinetics of the alteration products.

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 (see discussion in Chen et al., in press).

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. The models used in the sensitivity analysis must have enough of the important input parameters that the results become definitive. Regardless of the modeled results, it is clear that spent fuel alteration rate depends on the solution compositions, and this rate is critical to the radionuclide mobilization from the waste.

The effects of spent fuel dissolution on the attenuation of Np release are examined in a sensitivity analysis of the process-level model implementation for AREST-CT. In stage 1, the incorporation of Np into the secondary uranyl phases is analyzed based on the assumption that the Np concentration in the uranyl phases is the same as that in the spent fuel. In stage 2, models are used to calculate the dissolution rate of the secondary uranyl phases whose behavior is considered to be represented by a uranyl oxyhydroxide, schoepite. In fact, Np will be enriched or diluted in the secondary uranyl phases as compared with its original content in the spent fuel. This will depend specifically on the type of secondary minerals formed, the composition of fluid (especially the types of complex ligands, e.g., CO_3^{2-}), and the concentration of Np in fluid which largely depends on its release rate from spent fuel as compared with the rate of removal (e.g., due to transport in the fluid as a dissolved or colloid species or the incorporation of Np into alteration phases). Tertiary uranium phases will inevitably form (as they do in natural occurrences and in laboratory experiments) in the stage 2 alteration. Therefore, to some extent the Np released from the secondary phases will be retarded by incorporation into the tertiary uranium phases.

Concerning the formation of these secondary uranyl phases, the geochemists and analysts in the project are well aware of the limitations and difficulties of modeling these processes. The project's own list of uncertainties (CRWMS M&O, 1998c, Chapter 4, 4-93 to 4-94) is prescient. Among the cited uncertainties are:

1. The thermochemical and kinetic properties of the uranyl minerals are generally unknown.
2. The effects of the "basket" material corrosion on water chemistry are not considered in the model.
3. Radiolysis effects on corrosion of the waste forms are not considered. As we noted in the Panel's third interim report (Whipple et al., 1998), radiolysis can have important effects on the near-field, particularly for breached waste packages. Gamma radiation dose rates may be as high as 10^4 rad/hr at the surface of the canister. Radiolysis of water within a failed waste package can lead to the production of H_2 and O_2. Radiolytically produced H_2O_2 can lead to the formation of H_2O and O_2. Finn et al. (1996) have suggested that hydrogen peroxide may be responsible for a highly oxidizing environment during the corrosion of spent fuel. 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.
4. The effects of variations in flow rate and water composition have not been analyzed or examined by appropriate experiments.

5. The assumption of a porous-medium behavior has not been evaluated or confirmed experimentally.

In-Drift Colloid Model

The estimates of the concentration of "in-drift" colloids are based on a method similar to that used to estimate the incoming colloid concentration. The difference is that the incoming colloids are considered to be clay colloids, while the in-drift colloids are presumed to be dominated by iron-oxide colloids.

See section IV.G for a discussion of colloid formation, stability and transport.

In-Drift Microbial Communities Model

The analysis of microbial activity in the near-field environment was judged by the Panel to be at a preliminary stage. The project analysts are to be complemented about two aspects of the treatment: (1) the use of information from other national programs, e.g., Switzerland, and (2) the effort to compare modeled results (using MING) with results from the Swiss model.

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. As an example, the effort to bound the microbial growth, as a function of biomass production based on either energy limitations in the system or nutrient supply limitations to the microbes, requires important, perhaps unknowable, assumptions. One assumption, release rates of Fe^{2+} from biotite, requires further assumptions concerning the weathering of biotite (an Fe-bearing silicate) and its estimated lifetime (a lifetime of 1 million years was used as a conservative figure). Calculated cases included estimates of the lifetimes of other materials in the drifts (e.g., concrete, CRM and CAM). These assumptions are then incorporated into calculations that require temperature, infiltration rate and relative humidity values. In addition, variable groundwater compositions are utilized. 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.

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.

APPENDIX B: PEER REVIEW PLAN

Peer Review Plan for
the Performance Assessment Peer Review

Revision 03
January 29, 1999

Prepared by: ______________________________
Thomas E. Rodgers, Peer Review Coordinator
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Approved by: ______________________________
Chris G. Whipple, Peer Review Chairperson
ICF Kaiser Engineers, Inc.

(The original is signed)

Statement of Work

The objective of the Performance Assessment Peer Review is to provide a formal, independent evaluation and critique of the Total System Performance Assessment-Viability Assessment (TSPA-VA) for the Civilian Radioactive Waste Management System Management and Operating contractor (M&O).

Scope of the Review

The TSPA-VA will be conducted by the M&O for the U.S. Department of Energy (DOE) Yucca Mountain Site Characterization Office (YMSCO). The Peer Review Panel members will conduct a phased review over a two-year period to observe the development and completion of the TSPA-VA. The comments, concerns, conclusions, and recommendations of the final Peer Review Report will be provided to the M&O to support the development and conduct of the License Application TSPA (TSPA-LA). As such, the Panel members will consider not only the analytical approach of the TSPA-VA, but also its traceability and transparency.

The Panel members will evaluate the TSPA-VA for its analytical approach, including:

- physical events and processes considered in the analyses,
- use of appropriate and relevant data
- assumptions made
- abstraction of process models into the total system models
- application of accepted analytical methods
- treatment of uncertainties

These aspects will be evaluated within the context of their significance to the long-term performance of a repository at Yucca Mountain.

The traceability of the TSPA-VA refers to the extent to which a complete and unambiguous record exists of decisions, assumptions, models, and data, and their use in arriving at the results of the TSPA. Traceability is achieved through the documentation and explanation of how these four factors were used in the analyses.

Transparency means clear and logical documentation. A transparent TSPA will be clear not only to technical analysts, but also to other informed readers. An informed reader is one with an appropriate background in particular aspects such as the fundamental scientific and engineering principles, numerical analytical methods, or regulatory implications.

Quality Assurance

This peer review will be conducted in accordance with the requirements of M&O Quality Administrative Procedure (QAP) 3-3, Peer Review. The review will also be consistent with the guidance provided in the U.S. Nuclear Regulatory Commission's Generic Technical Position on Peer Review for High-Level Nuclear Waste Repositories (NUREG-1297).

Peer Review Group

The Peer Review Group consists of the six members of the Peer Review Panel, project personnel, and *ad hoc* consultants to the Panel.

Peer Review Panel

Six areas of technical expertise have been identified as necessary for a comprehensive review of the TSPA-VA and six Panel members have been selected to provide this expertise. In addition, one of the Panel members will serve as Chairperson. The expertise required and selected Panel members are:

- Chairperson and Risk Assessment - Dr. Chris G. Whipple
- Hydrology and Fluid Flow - Dr. Paul A. Witherspoon
- Physics and Nuclear Safety - Dr. Robert J. Budnitz
- Chemistry and Geochemistry - Dr. Rodney C. Ewing
- Biosphere and Health Physics - Dr. Dade W. Moeller
- Materials Science and Metallurgy - Dr. Joe H. Payer

A complete identification of the Panel members is provided in Appendix A.

Project Personnel

Responsible Manager – Mr. Jack N. Bailey, Director, M&O Regulatory and Licensing, is responsible for the conduct and completion of the TSPA-VA Peer Review.

Peer Review Coordinator – Mr. Thomas E. Rodgers, Senior Project Engineer, M&O External Interactions, will coordinate interactions between the M&O and the Peer Review Panel members.

Technical Secretary - Ms. Susan D. Wiltshire, M&O Planning and Communications Consultant, will facilitate interactions among the members of the Peer Review Panel and its consultants. She will have primary responsibility for documenting the activities of the Panel members.

Ad Hoc Consultants

The Panel Chairperson, with support from the M&O, may engage *ad hoc* consultants to provide technical advice to the Panel members on specific aspects of the review. These consultants may serve the Panel members where technical issues arise beyond the established expertise of the Panel members or where the volume of material to be reviewed requires technical support. The consultants will not have permanent standing on the Panel and will report their comments, concerns, conclusions, and recommendations through the appropriate Panel members. However, the consultants will meet the same quality assurance requirements as the Panel members. The Panel members will retain responsibility for assimilating all consultant work into the reports.

Comments, Concerns, Conclusions, and Recommendations

Members of the Panel will work interactively with the M&O and with all others who can contribute to the Panel's work. Panel members can request any information they deem necessary to the success of the review. Panel members will attend project meetings, technical exchanges, and workshops, as needed. They solicit advice concerning materials relevant to the review and welcome input from any group or individual.

Meetings and Interactions

The first and final meeting of each phase of the review (see Review Schedule Section) will be open. The final meeting of each phase will coincide with the first meeting of the succeeding phase in order to minimize the travel burden. Interactions at these meetings will be generally confined to the Panel members and those directly addressing them. The primary purpose of these meetings is to serve the needs of the Panel in gathering and interpreting information, in discussing various aspects of the TSPA as a group, and in planning future work. Time will be scheduled at each open meeting for the Panel to receive comments and questions from the public.

All other functions of the Panel, collectively and individually, will be treated as closed working sessions. The Panel member's geographic locations, other professional responsibilities, and the nature of the review itself dictate that they will conduct their review according to their own schedules. When multiple Panel members meet or interact among themselves about substantive topics, a meeting summary will be prepared and entered into the record of the review. When individual Panel members attend external meetings or engage in interactions or exchanges of information, the Panel members will prepare a written summary of the event and the information exchanged. These records will be entered into the permanent record of the review at the conclusion of each phase.

Reporting

At the conclusion of each of the first three phases, the Panel will prepare and deliver to the M&O an interim report presenting their comments, concerns, conclusions, and recommendations. The final phase of the review will conclude with the submittal of the final Peer Review Report. Each Panel member will contribute to the preparation of these reports. In addition, the Chairperson will prepare an executive summary highlighting key issues and noting the general progress of the review. The Panel members will present their findings to the M&O at the final meeting of each phase.

The Panel will report its comments, concerns, conclusions, and recommendations as a body. The Panel members will pursue agreement in their findings, but will not expect consensus among the diverse technical aspects of the review. Individual Panel members may include dissenting opinions, if they so choose.

The M&O will prepare letter responses to each of the three interim letter reports and a final response document for the Peer Review Report. These responses will document the disposition of each of the comments, concerns, conclusions, and recommendations made by the Panel members in their reports.

Review Schedule

The Performance Assessment Peer Review will take approximately two years to complete. The panel selection process began in October 1996, with the solicitation of nominations from the national and international technical communities. Panel selection was completed in January 1997. The review will formally commence in February 1997, and is expected to be completed by March 1999. The review will be conducted in four discrete phases:

Phase 1: TSPA Orientation - February to June 1997

The Panel members will be introduced to the high-level radioactive waste program, the YMSCO, and the performance assessment program. The Panel members will also familiarize themselves with the previous iterations of the TSPA (i.e., TSPA-91, -93, and -95) and related documents. The Panel members will consider the overall scope and approach planned for the TSPA-VA. Individual Panel members, by areas of expertise, will attend abstraction workshops and other pertinent PA interactions, and have access to all information necessary to initiate their review.

The Panel will conclude this phase with their first interim report on June 20, 1997.

Phase 2: Modeling, Scenarios, and Abstractions - June to December 1997

The Panel members will follow and review the process modeling, scenario development, and abstractions at a level of detail sufficient to permit them to engage in the subsequent review phases. The Panel members will also evaluate the methods, data, and assumptions that have been developed or identified for the Total System Performance Assessment to be used in the Viability Assessment. Interactions between the Panel members, the M&O PA organization, and other sources of expertise and information will continue.

The Panel will conclude this phase with their second interim report on December 15, 1997.

Phase 3: Draft TSPA Review - December 1997 to June 1998

The Panel members will observe and review the process of developing the draft TSPA-VA. They will review the draft documentation of abstraction activities, the preliminary results of the TSPA-VA, and the draft TSPA-VA document during this phase. Their comments, concerns, conclusions, and recommendations will be documented in the third interim report.

The Panel will conclude this phase with their third interim report on June 30, 1998.

Phase 4: Final TSPA Peer Review - July 1998 to January 1999

Panel members will be provided with copies of the final TSPA-VA report, once it has been completed, for their review. The Panel will also be provided copies of the final TSPA-VA

Technical Bases Document that contains supporting technical details on many aspects of the TSPA-VA. The Panel will document their comments, concerns, conclusions, and recommendations in the final Performance Assessment Peer Review Report.

The Panel will conclude this phase with their final Peer Review Report on February 12, 1999.

Review Criteria

Among the potential review criteria enumerated in QAP-3-3 (Section 5.2.2A), the following are most appropriate* to this review:

1. Validity of the assumptions

2. Alternate interpretations

3. Appropriateness and limitations of the methods and implementing documents

4. Accuracy of calculations

5. Validity of conclusions

6. Uncertainty of results

* The remaining potential review criteria enumerated in QAP-3-3 (Section 5.2.2A) are less appropriate to this review as follows:

7. Adequacy of requirements and criteria (review scope limited to technical evaluation of the appropriateness of the TSPA-VA)

8. Adequacy of application (selected criteria cover the intent of this criterion)

9. Qualification status of software used (verification and validation of computer software is outside the review scope)

In addition, review criterion 6 was revised to "uncertainty of results" from "uncertainty of results and impact if wrong" (the uncertainty in the TSPA-VA results, if wrong, can not be realistically evaluated in the absence of a regulatory standard)

(An Appendix to this Plan listing Peer Review Panel members addresses and phone numbers has not been included, because this list is provided in the following Appendix)

APPENDIX C: PEER REVIEW PANEL

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ACRONYMS AND ABBREVIATIONS

CFR	Code of Federal Regulations
CRM	corrosion resistant metal
CRWMS	Civilian Radioactive Waste Management System
DOE	U.S. Department of Energy
DKM	dual permeability model
EBS	Engineered Barrier System
Eh	Oxidizing potential
ICRP	International Commission on Radiological Protection
LA	License Application
M&O	Management and Operating Contractor
NFGE	Near-field geochemical environment
PSHA	Probabilistic seismic hazard analysis
PVHA	Probabilistic volcanic hazard analysis
SZ	Saturated zone
TH	Themohydrology
THC	Thermohydrochemical
THM	Thermohydromechanical
THMC	Thermo-hydrological-mechanical-chemical
TSPA	Total System Performance Assessment
TSPA-LA	TSPA to support a license application
TSPA-91, -93, -95	TSPAs completed in 1991, 1993, and 1995
TSPA-VA	TSPA supporting the Viability Assessment
USEPA	U.S. Environmental Protection Agency
USNRC	U. S. Nuclear Regulatory Commission
UZ	Unsaturated zone
VA	Viability Assessment
WP	Waste Package

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