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Total System Performance Assessment - Viability Assessment (TSPA-VA) Methods and Assumptions

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Civilian Radioactive Waste Management System

Management & Operating Contractor

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Winston & Strawn
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Prepared by:
TRW Environmental Safety Systems Inc.

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1000 Independence Avenue, S.W.
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Prepared for:

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

Prepared by:

TRW
1180 Town Center Drive
Las Vegas, Nevada 89134

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Prepared by:

R. W. Andrews
R. W. Barnard
H. A. Dockery
J. H. Gauthier
J. A. McNeish
S. D. Sevougian
M. L. Wilson

With Contributions from:

S. J. Altman, B. W. Arnold, N. D. Francis, C. K. Ho, J. H. Lee,
J. E. Houseworth, R. L. Howard, D. C. Sassani,
E. R. Siegmann, A. J. Smith, S. Steward, and J. J. Tappen

Reviewed by: ______________________ **Date:** November 12, 1997
Robert W. Andrews, Manager
Performance Assessment & Modeling

Approved by: ______________________ **Date:** 11-13-97
J. L. Younker, Manager
Regulatory Operations

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Individuals who provided review of or additions to various sections of the document and are not listed as section authors include: Bo Bodvarsson (M&O/LBNL); William Halsey (M&O/LLNL); William Glassley (M&O/LLNL); Bruce Robinson (M&O/LANL); George Barr (M&O/SNL); Patrick Tucci (USGS); and Ray Stout (M&O/LLNL).

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EXECUTIVE SUMMARY

Yucca Mountain, in southern Nevada, is under consideration by the U.S. Department of Energy's Office of Civilian Radioactive Waste Management, Yucca Mountain Site Characterization Office (YMSCO) as a potential site for the Nation's nuclear waste repository. The DOE is investigating the feasibility of permanently disposing the Nation's commercial high-level radioactive wastes (in the form of spent fuel from the over 100 electric power-generating nuclear reactors across the U.S.) and a portion of the defense high-level radioactive wastes (currently stored at federal facilities around the country) in the unsaturated volcanic rocks underlying Yucca Mountain, Nevada. For convenience, the work done by the YMSCO organization will be referred to as the Yucca Mountain Project hereafter.

The goal of the Yucca Mountain Project is to produce the analyses and documentation to support, by the year 2002, submission of a License Application to construct a repository at the Yucca Mountain site. An interim step in this process, as defined by the Yucca Mountain Project Program Plan is the completion of a Viability Assessment in 1998. A principal objective of the Viability Assessment is to address the major unresolved technical questions so that an informed judgement can be made concerning the viability of licensing and constructing a geologic repository at the Yucca Mountain site. This objective requires the completion of the following tasks:

- Development of the preliminary design concept for the critical elements of the repository and waste package;

- Completion of 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;

- A plan and cost estimate for the remaining work required to complete a license application; and

- An estimate of the costs to construct and operate the repository in accordance with the design concept.

This report provides a roadmap of the general methodology and approach for implementing the second task shown above, i.e., completion of a total-system performance assessment for the viability assessment (TSPA-VA). The TSPA-VA will be the fourth in a series of iterative performance assessments conducted by Yucca Mountain Project. It will build and improve on the knowledge gained from all of the previous analysis efforts and it will incorporate the most current Yucca Mountain Project design concepts and analyses of available site and engineering data. The ultimate goal will be to provide the most defensible model of long-term total system behavior for Yucca Mountain in support of the viability decision.

Total-system performance assessment is an analysis in which all significant features, events, and processes are represented in models of appropriate levels of complexity to estimate behavior of the system and to compare this behavior against specified performance standards. In the case of the potential Yucca Mountain repository system, a TSPA must capture all of the important components of both the engineered and the natural system. In addition, a TSPA must evaluate the overall uncertainty in the prediction of waste containment and isolation, as well as the risks caused by the uncertainty in the individual component models, and corresponding parameters.

Total-system performance assessments serve at least two purposes. First the TSPA provides the basis for predicting system behavior and evaluating that behavior against safety measures (in the form of regulatory standards.) Second, the results of TSPA analyses and sensitivity studies also provide guidance to site characterization and repository design activities in terms of prioritizing the most important tests and selecting the most effective design options.

The present document focuses on the overall approach to be followed—an approach that will ensure that the most current understanding can be embodied in the TSPA-VA and that a representative suite of conceptual model and parameter uncertainties will be addressed for each component. The overall approach to TSPA-VA may be broken into the following eight activities:

1. Develop, substantiate, test, and document models of all relevant processes affecting post-closure waste containment and isolation, using input from scientific and design investigations.

2. Identify relevant uncertainties in process models.

3. Identify all relevant scenarios to be analyzed in the total system performance assessment.

4. Conduct sensitivity analyses on each of the key process models to determine the effects of all of the relevant uncertainties.

5. Abstract the relevant results from the process models (including the uncertainty) to provide input to the total system model.

6. Conduct total system analyses that will predict performance.

7. Document all assumptions, results, and conclusions including those relevant to the prioritization of future site and design activities required to develop a more robust analysis for the License Application.

8. Conduct a Peer Review of the TSPA assumptions, results, and conclusions.

The components of the Yucca Mountain repository system include five major elements that must be evaluated : (1) the natural environment unperturbed by the presence of underground openings or emplaced wastes, (2) the perturbations in the natural system caused by the construction of the underground facilities and the emplacement of wastes, (3) the long-term degradation of the engineered components designed to contain the radioactive wastes, (4) the release of the radionuclides from the engineered containment system, and finally (5) the migration of these radionuclides through the engineered and natural barriers to the biosphere and the ultimate uptake by plants, animals and humans leading to a dose consequence. Although the processes that operate in these five elements are interrelated, in order to more reasonably model the complexity of the system, PA has developed the following subdivisions that will comprise the TSPA-VA analysis models:

- Precipitation
- Net Infiltration
- Unsaturated Zone Flow
- Mountain-Scale Thermal Hydrology
- Drift-scale Seepage
- Drift-Scale Thermal Hydrology
- Drift-Scale Thermal Chemistry
- Waste-Package Degradation
- Cladding Degradation
- Waste-Form Degradation
- Radionuclide Mobilization
- Radionuclide Transport in the Engineered Barriers
- Radionuclide Transport in the Unsaturated Zone
- Radionuclide Transport in the Saturated Zone
- Radionuclide Transport in the Biosphere
- Disruptive Events: Volcanism, Tectonism, Criticality

These processes are all included in the Yucca Mountain Project Waste Containment and Isolation Strategy and also are directly related to Key Technical Issues important for assessing the long-term safety of a potential Yucca Mountain repository, as defined by the U.S. Nuclear Regulatory Commission. For the final TSPA-VA calculations, these processes and associated models (each with a different degree of detail based on current knowledge), will be recombined and run as a composite system.

This document presents the details of the planned TSPA-VA method for modeling each of the above individual processes, including uncertainty, and the approach for combining them into an overall model and computer code. The presentation contains a detailed discussion of the process-model basis for each of these major components of TSPA-VA. As an overview, we describe how each component was handled in previous TSPAs and what is currently known about the component. Issues important to understanding the component, as determined during workshops involving Yucca Mountain Project participants and other knowledgeable members of the scientific community, are presented next. Then we discuss how the component will be abstracted (modified and/or simplified) for use in TSPA-VA, including what assumptions are made that could affect the results. Finally, we outline how the component will be treated in the TSPA-VA "base-case," and what sensitivity analyses will be conducted to examine alternative models of the component, and uncertainties in parameters not considered in the base case.

In general terms, the approaches to be used for the major components for TSPA-VA are as follows:

- Unsaturated-zone flow is modeled directly with the Yucca Mountain Project-developed 3-dimensional site-scale unsaturated zone-flow model, using a finite-difference computer program named TOUGH2. Seepage of water into emplacement drifts is modeled with a response-surface method, using information from unsaturated zone flow and thermohydrology. Climate change is modeled within TSPA calculations by assuming a series of step changes in boundary conditions.

- Mountain-scale unsaturated-zone thermohydrology is modeled with 2-dimensional cross sections and 1-dimensional columns taken from the 3-dimensional site-scale unsaturated zone-flow model, using the TOUGH2 computer program. Drift-scale unsaturated-zone thermohydrology is modeled with a finite-difference computer program named NUFT in 3-dimensions using a model domain that contains eight waste packages, and stretches from the water table to the ground surface vertically.

- Near-field geochemical environment (i.e., drift-scale thermal chemistry) is modeled in the TSPA calculations with a response-surface of various chemical composition parameters, generated by multiple simulations of in-drift geochemistry models, using geochemical reaction-path (EQ3/6) and reactive-transport (AREST-CT) software programs.

- Waste-package and drip-shield degradation are modeled using a computer code named WAPDEG, which includes both variability on a given package and variability from package-to-package. The results are used as response surfaces in the TSPA-VA calculations, representing distributions of waste-package initial failure times and progress of degradation (corrosion) with time.

- Waste-form and cladding degradation are modeled within the executive TSPA "driver" program, Repository Integration Program (RIP), using empirical degradation-rate formulas developed from available data.

- Engineered-barrier-system transport is modeled within RIP, using the RIP cells algorithm, based on an idealized representation (basically a linked series of equilibrium batch reactors) of waste form, waste package, corrosion products, and invert, and how radionuclides move through them.

- Unsaturated-zone radionuclide transport is modeled directly with the Yucca Mountain Project-developed 3-dimensional site-scale unsaturated zone-transport model, using a finite-element computer program named FEHM.

- Saturated-zone flow and transport are modeled using a convolution method, with the convolution kernels developed with the Yucca Mountain Project-developed 3-dimensional site-scale saturated zone-flow-and-transport model, which uses the FEHM computer program.

- Biosphere is modeled within TSPA calculations using biosphere dose-conversion factors, which convert SZ radionuclide concentration to individual radiation dose. The biosphere dose conversion factors are developed using a computer program named GENII. The individual doses are the end product of the TSPA calculations.

- Disruptive events to be considered are seismic activity, igneous activity, nuclear criticality, and human intrusion. The probability of events is modeled within RIP, and the consequences are modeled by making modifications of the affected TSPA components.

Based on the "base-case" definitions of these various component models, an overall "base-case" TSPA-VA model will be constructed. This represents an assessment of the most likely range of behavior for the overall repository system. This is essentially a combination of the most likely ranges of behavior for the various component models, processes, and corresponding parameters. In addition to the base-case repository performance, behavior that is considered less likely is captured in the "sensitivity cases" for alternative models and parameter ranges of the various processes. Other sensitivity cases examine the effect of alternative repository designs.

We will represent the TSPA-VA results in two main forms: (1) probability distributions (e.g., complementary cumulative distribution functions) for peak dose to a receptor 20 kilometers down gradient of the repository, and (2) time histories of the peak dose at 20 kilometers down gradient over the expected life of the repository. These distances are chosen based on the Interim YMP Post-Closure Performance Goal. A realization near the mean or median of the appropriate CCDF will be used to define the most probable time-history for future repository behavior for both the base case and for the combined base case and sensitivity studies.

Various sensitivity analysis methods (uncertainty importance analysis) for determining the most influential system parameters will be presented. This will include methods for displaying the results in a way that most transparently demonstrates the key natural- and engineered-barrier parameters and features. This helps in prioritizing future site-characterization efforts and best possible design options.

This document provides a detailed description of the overall TSPA-VA model architecture, based on the various forms of abstractions used for the component models, such as spatial-domain-based abstractions, process-based abstractions, dimensionality abstractions, and response-surface abstractions. This leads to a description of the computer code architecture, including a delineation of how the input/output of the various codes (mentioned above) will be connected.

In conclusion, quantitative total-system performance assessments based on the most current understanding of the processes and parameters potentially affecting the long-term behavior of the disposal system will be used to assess the viability of the Yucca Mountain site and its associated engineered designs in terms of its predicted ability to meet overall system performance standards. The present document summarizes the current status of the approach, methods, and key assumptions that are intended to be used in TSPA-VA. This document effectively serves as a preliminary draft introductory chapter for the TSPA-VA document to be completed in the summer of 1998.

1.0 VIABILITY ASSESSMENT FOR YUCCA MOUNTAIN

Holly A. Dockery

The U.S. Department of Energy (DOE) is investigating the feasibility of permanently disposing the nation's commercial high-level radioactive wastes (in the form of spent fuel from the over 100 electric power-generating nuclear reactors across the U.S.) and a portion of the defense high-level radioactive wastes (currently stored at federal facilities around the country) in the unsaturated volcanic rocks underlying Yucca Mountain, Nevada. Quantitative performance assessments based on the most current understanding of the processes and parameters potentially affecting the long-term behavior of the disposal system are to be part of the information available for judging the viability of the site and its associated engineered designs.

1.1 HISTORY OF THE YUCCA MOUNTAIN PROJECT

1.1.1 Site Selection

Yucca Mountain, Figure (1.1-1), located in southwestern Nevada, has been the subject of investigations concerning its suitability as a site for a mined geologic repository system for the disposal of radioactive waste for almost two decades. Some of the alternatives other than geological disposal, considered as methods for permanent storage of U. S. radioactive waste, include disposal in very deep boreholes, on islands, in continental ice sheets, into space, into the subseabed, or by transmutation. DOE (1980) discusses these and other methods of disposing of radioactive waste from the commercial sector. However, due to technical, environmental and feasibility considerations, deep geologic disposal of commercially generated radioactive wastes has been the official policy of the United States since 1982 (Public Law 97-425).

In 1980, a program was organized to identify potential U.S. sites appropriate for disposal of spent power-reactor fuel and high-level-radioactive waste. The sites identified included ones that had been previously restricted to federal governmental use (the Hanford Site in Washington and the Nevada Test Site) and also those with large regions underlain by potentially suitable rock types (mostly rock salt and granitic rocks). The list of sites developed by this program included Hanford, Washington; Yucca Mountain, Nevada; Davis Canyon and Lavender Canyon, Utah; Deaf Smith and Swisher counties, Texas; Vacherie dome, Louisiana; and the Cypress Creek and Richton domes, Mississippi. In 1982, the Nuclear Waste Policy Act initiated evaluation of the sites listed above for use as the first repository to contain 70,000 metric tons of uranium reactor fuel and radioactive waste. (A program to identify a second repository site, primarily in granite, was also ongoing at the time, although no specific sites were identified for investigation). On the basis of these evaluations, three sites were selected for detailed characterization: Hanford, Deaf Smith, and Yucca Mountain. Finally, in 1987, Congress determined that all resources related to evaluating repository sites would be focused on Yucca Mountain. Efforts at Hanford, Deaf Smith, and for the second repository were halted. This directive is contained in the Nuclear Waste Policy Amendments Act of 1987 (Public Law 100-203).

1.1.2 Evolution of Regulatory Guidance

The Nuclear Waste Policy Act of 1982 (Public Law 97-425, 1982) set forth the basic policy for approving a site for disposal of radioactive waste. General siting guidelines were defined by the DOE in 10 CFR Part 960. These guidelines included a number of criteria related to "favorable" or "unfavorable" characteristics against which a specific site could be evaluated. Conclusions about a site based on these criteria could result in a finding of unsuitability (a disqualifying condition is present or a qualifying condition is not present) or suitability (disqualifying conditions are not present or qualifying conditions are present).

Levels of suitability findings were also defined. Lower level findings were primarily to be used for screening of multiple sites. Higher level findings were primarily to be used for recommending a single site from among three sites for development of a geologic repository. A lower-level suitability finding could be made if a conclusion concerning the presence or absence of a condition could change with additional information. Conversely, a higher-level finding was supported when new information was unlikely to change the conclusion. A detailed preliminary evaluation of the Yucca Mountain using these criteria was documented in Younker, et al. (1992). The finding of that analysis, based on the models and data available at the time, was that "none of the disqualifying conditions are present or likely to be present" and that, at a minimum, "lower level suitability findings can continue to be supported for the qualifying conditions for all of the Postclosure Guidelines." Lower level findings were rendered irrelevant by the 1987 amendments to the Nuclear Waste Policy Act.

If a formal determination of suitability had been made, DOE could have proceeded with the site recommendation process followed by a License Application (LA) to construct and operate a high-level radioactive waste repository. At that point, the Nuclear Regulatory Commission (NRC) would have assessed whether or not the analyses in the LA indicated compliance with regulations contained in 10 CFR Part 60. This regulation covers all aspects of repository siting, design, operation, and post-closure performance. In general, this standard requires that the repository system: (1) not exceed a cumulative 10,000-year release normalized by the Environmental Protection Agency (EPA) release limits at the accessible environment (AE), (2) meets EPA standards for individual and groundwater protection, (3) provides reasonable assurance of "substantially complete" containment of waste by the waste packages for a period of 300 to 1000 years, (4) meets a prescribed limit on release rate from the engineered barrier system (EBS), and (5) demonstrates a 1000-year or greater pre-waste-emplacement groundwater travel time along the "fastest path of radionuclide travel" to the AE. The AE was defined as being the ground surface, and the subsurface at a distance of up to 5 km from the edge of the repository.

However, regulations governing performance of Yucca Mountain set forth by the EPA in 40 CFR 191 were remanded by the Energy Policy Act of 1992 (Public Law 102-486, 1992). The Act mandated a separate process for setting a standard specifically for Yucca Mountain. The EPA was directed to retain the National Academy of Sciences (NAS) to formulate a recommendation for a new standard that "shall prescribe the maximum annual effective dose equivalent to individual members of the public from releases to the accessible environment from radioactive materials stored or disposed of in the repository". The next step was for the EPA to repromulgate their standard within one year of the NAS recommendation, taking into consideration those recommendations. Further, the NRC was also directed to revise its requirements consistent with the resulting new EPA requirements. This process is ongoing and no new standard for a Yucca Mountain repository has been promulgated to date.

Previous total system performance assessments (TSPAs) have focused in part on assessment of the repository system against these remanded regulations. However, in anticipation of expected changes to the requirements, TSPAs performed in 1993 (Wilson, et al., 1994; Andrews, et al., 1994) and 1995 (M&O, 1995) explored performance measures related to individual drinking water dose rates. The analyses were also run for much longer time periods (up to 1,000,000 years after closure) to capture the occurrence time for peak dose attributable to certain radionuclides.

1.1.3 Performance Measures for TSPA-VA

The performance measures adopted for any total system analysis drive the relative importance of individual features, processes, and parameters. There are several alternative performance measures which may be selected to evaluate the system, including dose to a hypothetical individual, or to a member of a particular population (critical group), or cumulative release to a particular location. Largely in support of the design process, an interim postclosure performance measure was developed for use within the Yucca Mountain Project (Barnes, 1997). The YMP interim performance measure suggests evaluating expected dose to an average individual in a critical group living 20 km from the repository. While the DOE believes that the appropriate point of compliance, based on current-day characteristics of the region, should be at 30 km downgradient from the repository, 20 km was selected to provide additional conservatism. The time period of interest for the analyses will be primarily 10,000 and 100,000 years, with minimal analyses of a 1,000,000 year time period.

1.2 EVOLUTION OF CURRENT PROGRAM PLAN

A very large body of information has been collected for the Yucca Mountain potential repository site and its engineered components. An early synthesis of such studies of the site is contained in the Environmental Assessment (DOE, 1986). The Site Characterization Plan (SCP) (DOE, 1988) further expanded this information. The SCP also laid out a strategy that required completion of a detailed set of activities that was expected to provide all of the information needed to comprehensively describe the repository system. It also documented methods for assessing the performance of the total repository system, as well as all of the individual components. Until 1996, the DOE Yucca Mountain Site Characterization Program (YMP) strategy followed the plans contained in the SCP, although several efforts were made to help prioritize the massive number of recommended studies (Test Prioritization Task, Mattson, et al, 1991; Integrated Test Evaluation, Younker, et al., 1992).

In 1996, YMP revised this program strategy consistent with the guidance provided by the President and the Congress (DOE, 1996). The goal of submitting a successful license application to the Nuclear Regulatory Commission, however, remained central to the Program's mission. The strategy required that YMP identify, prioritize, and schedule a focused set of site characterization activities that would allow submission of a License Application for construction authorization in 2002. The strategy also called for a Viability Assessment (VA) to address by 1998 the major unresolved technical questions so that an informed assessment could be made of the viability of licensing and constructing a geologic repository at the Yucca Mountain site (DOE, 1996). The VA was anticipated to be an integral step on the path to a license application.

This strategy represented a significant change in philosophy when compared to that defined by the SCP. The expectation by the authors of the SCP was that the entire suite of proposed activities would be completed because only limited performance assessment results were available at that time to help discriminate among the various processes in terms of relative importance. However, the VA strategy allows YMP to concentrate its resources on studying those features, processes, and parameters likely to have the strongest influence on long-term system performance.

After completion of the VA in 1998, YMP will prepare the additional information required for the Secretary of Energy's Site Recommendation to the President and for the License Application to the Nuclear Regulatory Commission. As part of the Site Recommendation and License Application process, a Draft Repository Environmental Impact Statement (EIS) will be submitted for public review and comment in 1999. The Final Repository EIS and Record of Decision will be submitted in 2000. If the site is found suitable, public hearings will be conducted by YMP in the state of Nevada. The Secretary will then issue a Site Recommendation in 2001. The decision on Site Recommendation will be based on the data obtained from site characterization, a description of the proposed repository and waste package, the Final Repository EIS, preliminary comments from the Nuclear Regulatory Commission on the sufficiency of information for licensing, the views and comments of the public, the AUGs, and the State of Nevada, and other relevant information required by the Nuclear Waste Policy Act, as amended. If the site is approved, YMP will submit a license application in 2002. This schedule will allow YMP to meet the long-term goal of starting repository emplacement operations in 2010.

1.3 OBJECTIVE OF THE VIABILITY ASSESSMENT

A principal objective of the VA is to address, by 1998, the major unresolved technical questions so that an informed assessment can be made concerning the viability of licensing and constructing a geologic repository at the Yucca Mountain site. This objective requires the completion of certain tasks, including:

(1) development of the preliminary design concept for the critical elements for the repository and waste package;
(2) completion of 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;
(3) a plan and cost estimate for the remaining work required to complete a license application; and
(4) an estimate of the costs to construct and operate the repository in accordance with the design concept.

The main objective of the TSPA-VA is to incorporate the most current site and design information into a defensible representation of the probable long-term behavior of a potential repository system at Yucca Mountain. This representation, however, includes alternative conceptual models, variability and uncertainty in parameters and processes, and a sufficient level of detail to represent the aspects of each process that are important to performance. TSPA-VA will also provide an evaluation concerning the degree of safety the system is expected to provide to the public. This information will serve as the performance assessment input to allow a judgement regarding the viability of the Yucca Mountain Project.

The TSPA-VA is also expected to be a "dry run" for the analyses used to support further work leading toward the license application (LA). TSPA-VA will be rigorously reviewed by internal and external review groups and by the NRC. Feedback from these reviews will be incorporated into the development and implementation of the TSPA-LA. In addition, the TSPA-VA will also provide guidance for what information is needed from site characterization and design activities in order to adequately support the development of models underlying the TSPA-LA.

1.4 OBJECTIVE OF THIS REPORT

As shown above, the second component of the viability assessment will be an updated total system performance assessment (TSPA) based on YMP design concepts and the analyses of available site and engineering data. This report provides a roadmap of the general plan for implementing a total-system performance assessment for the VA (TSPA-VA). In addition, this document effectively serves as a preliminary draft of an introductory chapter for the TSPA-VA document, which will be completed in the summer of 1998.

Chapter 2. This chapter discusses the plans, objectives, and schedule for the TSPA-VA.

Chapter 3. The historical perspective of TSPA-VA is provided in this section. The key events and previous performance assessments are summarized.

Chapter 4. The key components of the TSPA are described in this section. The base case design is presented. How the potential repository system is expected to work, what analyses are being conducted for TSPA-VA, and how the TSPA aligns with the NRC's Key Technical Issues (KTIs) and DOE's Waste Containment and Isolation Strategy (WCIS) are presented.

Chapter 5. The overall general approach and method to producing the analyses for TSPA-VA is presented in this section. The activities in FY97 leading up the TSPA-VA analyses are described, along with a brief discussion of the abstractions (i.e., model simplifications) to be used in TSPA-VA.

Chapter 6. This chapter is the largest in the document and it describes the key model abstractions to be used in the TSPA-VA. The results from the integration workshops held in FY97 are presented, along with the planned base-case and sensitivity-case analyses to be conducted for TSPA-VA for each of the component models.

Chapter 7. A more detailed look at the base case model and its implementation is provided in this chapter. The information flow, code architecture, and model architecture are presented. Additionally, the planned treatment of uncertainty and variability is presented, along with more detail on the sensitivity analyses to be conducted.

Chapter 8. A summary of the TSPA-VA is provided in this section. The range of users of the TSPA-VA information, key cross-cutting technical issues, and general philosophy of TSPA-VA are summarized in this section.

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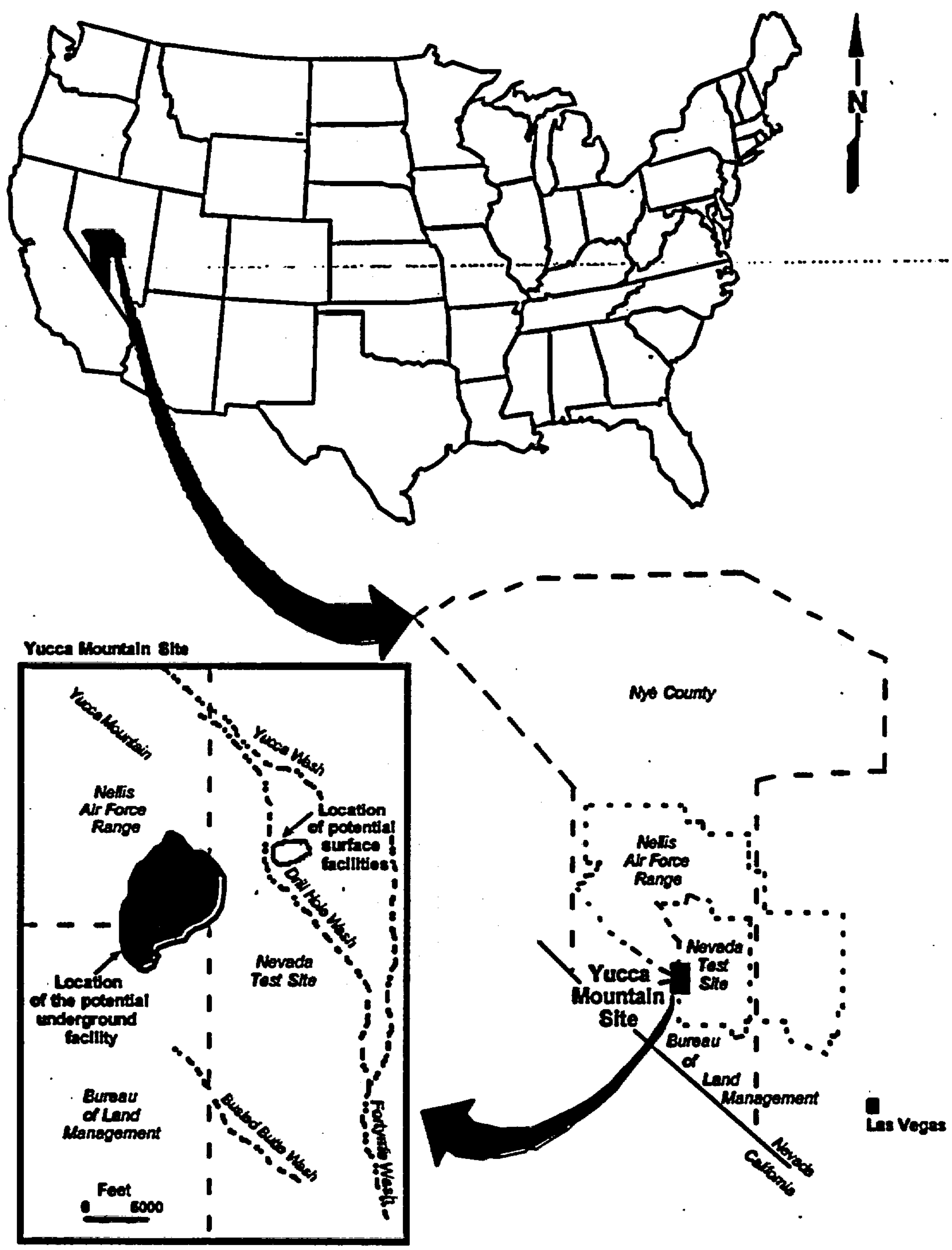

Figure 1.1-1. Location Map of Yucca Mountain Potential Repository Site

2.0 TSPA-VA

Holly A. Dockery

2.1 DEFINITION OF TSPA

Total-system performance assessment is an analysis in which all significant features, events, and processes (FEPs)[1] are represented in models of appropriate level of complexity, (discussed in more detail in Section 2.3.1) to estimate behavior of the system and to compare this behavior against specified performance standards. In the case of the potential Yucca Mountain repository system, a TSPA must capture all of the important components of both the engineered and the natural system. In addition, a TSPA must evaluate the uncertainty in the prediction of waste containment and isolation, as well as the risks associated with waste isolation caused by the uncertainty in the individual component process models and parameters.

Total system performance assessments serve many purposes. They provide integrated evaluations of the overall system that can be used to compare with regulatory and other requirements. They inform judgements about the relative importance of information-gathering activities in site characterization and about areas of particular importance for design of the engineered system. In addition, the assessments can be used to assist in a site recommendation which may ultimately lead to licensing. Also, sensitivity studies conducted as part of the assessment help to identify those barriers and processes of most importance to total system performance.

This process of total system analysis is iterative, meaning that incorporation of revised and updated information into subsequent TSPAs allows a progression toward more reasonable and defensible total-system models. The evolution of this process for the potential Yucca Mountain repository is described in more detail in Chapter 3.

Many of the individual components of the YMP TSPA analyses correspond to attributes in the U.S. DOE's Waste Containment and Isolation Strategy (WCIS) (DOE, 1996) including: (1) rate of water seepage into the repository, (2) waste-package lifetime (containment), (3) rate of release (mobilization) of radionuclides from breached waste packages, (4) radionuclide transport through engineered and natural barriers, and (5) dilution in the saturated zone below the repository. Each one of the attributes in the WCIS will be evaluated by the TSPA-VA to determine, first, if the component operates as expected in the context of the total system, and second, how much each component contributes to the overall safety of the system and thus to the ability of YMP to demonstrate safety with an in-depth defense.

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[1] Features are the geologic or hydrologic properties of the site or system, which are expected to be enduring. Processes are phenomena that have gradual, continuous interactions with the system. Events are occurrences that have a specific starting time, and usually a duration shorter than the time being simulated. (See Sections 5.2.3 and 6.10)

2.2 PLAN AND SCHEDULE FOR THE TSPA-VA

Planning of the TSPA-VA began in late FY96 and was reported in the TSPA-VA Plan (M&O, 1996). The general plan included steps for developing and enhancing the "abstracted" (i.e., reduced computational time) models[2] for the various components of a TSPA and also for developing and implementing the overall methodology and approach for the total-system modeling (see Chapter 5, this report). However, information feeding TSPA models is rapidly evolving as new site and laboratory data are collected and interpreted. Changes to the potential repository system analyses also occur as design alternatives are explored, incorporated, and/or discarded. Because of the highly coupled nature of the engineered and natural components of the system, changes to any one system component are likely to change the response of many other system components. Therefore, the plan developed for the TSPA-VA included the flexibility to constantly assess, reprioritize, and alter modeling activities to ensure the best possible product. However, the TSPA process, which includes developing appropriate models and parameters, running TSPA analyses, and interpreting and documenting results, is a time and resource intensive set of activities. Thus, when the site characterization and design information that feed the TSPA models are frozen for the TSPA-VA analyses in Fall 1997, there will be some newer information that will not be included in the TSPA-VA, but will be captured in the TSPA-LA.

A large part of the effort associated with the TSPA-VA activity is directed toward developing abstracted models for use in the probabilistic TSPA, in order to describe the different natural and engineered components of the total system. Another major effort is associated with combining these components into a representation to allow prediction of "probable behavior". This representation, however, includes alternative conceptual models, variability and uncertainty in parameters and processes, and a sufficient level of detail to represent the aspects of each process that are important to performance. Thus, even though a major part of the TSPA effort includes "abstracting" information into the simplest form reasonably possible without losing the key sensitivities in the process model, the models used to calculate probable behavior necessarily retain a great deal of complexity.

2.2.1 Abstraction/Testing Activities

The difficulty in handling the complexity of the repository system in a single analysis leads to a discretization of the various components of the Yucca Mountain total system into individual process areas, or domains. The process areas that formed the topic of each abstraction/testing activity for TSPA-VA are: unsaturated zone flow, thermohydrology, near-field geochemical environment, waste-package degradation, waste-form alteration and mobilization, unsaturated-zone transport,

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[2]The abstraction of process model results is the method of simplifying the essential components of the process model in a suitable form for use in an assessment of total system performance. The simplification should retain the basic intrinsic form of the process model without requiring the complexity incorporated in the process model. Such model abstraction is required in order to maximize the utilization of finite computational resources while allowing a sufficient range of sensitivity and uncertainty analyses.

saturated-zone flow and transport, biosphere, and disruptive events (volcanism, seismicity, human intrusion, and nuclear criticality). Although there is significant coupling between many of these process models, they can be treated separately for the analysis by rigorously maintaining a consistent set of boundary conditions and scenarios. A significant part of the abstraction (i.e., model simplification) activities has focused on maintaining these relationships and sequencing the results of the activities so that input and output to the various models is available at the appropriate time and in the appropriate form.

Workshops and Analyses. A series of abstraction/testing workshops was conducted between December, 1996 and June, 1997. These workshops brought investigators from YMP PA, Site, and Design organizations together to identify and prioritize issues related to each process that should be addressed in TSPA-VA. In addition to the workshop participants, observers at the workshops included NRC staff, members of the TSPA-VA Peer Review team, representatives of DOE-EM, the EIS contractor and EPA contractors. These observers provided comments, but the responsibility of identifying and prioritizing the issues was with the participants.

The workshop participants developed plans to construct abstractions of each major process. These abstractions are designed to address the top priority issues and incorporate the most current project understanding into the models. The results of each workshop were documented in deliverables that were completed approximately six to eight weeks after the conclusion of each workshop (M&O, 1997a; M&O, 1997b; M&O, 1997c; M&O, 1997d; M&O, 1997e; M&O, 1997f; M&O, 1997g, M&O, in press-a, M&O, in press-b).

The efforts to develop the abstracted representation of each component/model, as defined in the various aforementioned deliverables, are currently ongoing but are expected to be completed by mid-November, 1997 (see Figure 2.3-1). At that point, the abstractions will be fed into the TSPA-VA base case (described in Chapters 6 and 7). Sensitivity analyses will be conducted on each of the abstraction components to investigate uncertainties in key site and design parameters, as well as alternative conceptual models not included in the base case analyses.

Status Meetings and Preliminary Documentation. In the course of the abstraction/testing activities, several status meetings have already been conducted to assess progress, ensure integration, and to adjust the analyses, as needed. These meetings have been attended by PA, site, and design analysts and managers, as well as DOE personnel and PA Peer Review Panel members. Additional informal meetings are scheduled in early September, 1997 for the same reasons stated above. A more formal status presentation will be held in April, 1998 to present initial results of the sensitivity analyses run on the base case. This presentation will provide an opportunity for DOE, the PA Peer Review panel, and other M&O organizations to have input on the analyses before they are completed.

The results and conclusions of all the model abstraction/testing activities feeding the base case will be documented in early 1998 as "preliminary chapters" of the TSPA-VA. The documentation will consist of: a comparison of the abstractions used in previous TSPA analyses and those to be used in TSPA-VA based on the current abstraction/testing; a description of the technical basis for all input assumptions and parameters; a description of the uncertainty in the conceptual representation; identification of the preferred conceptual models (where appropriate); documentation of the technical credibility/defensibility of the process model used in the abstraction; and discussion of the implications of the abstraction/testing results to additional design and/or site characterization activities. The documentation will be reviewed by appropriate M&O technical staff and review comments will be incorporated into the document. Each revised "preliminary chapter" will be used as part of the Draft TSPA-VA document, along with the documentation of the implementation and results of the sensitivity analyses run on the base case.

2.2.2 TSPA Activities

The activities associated with construction, implementation, and documentation of the TSPA-VA are described below (see also Figure 2.3-2). Although the activities are described here as being separate from those associated with the Abstraction/Testing activities, they are, in fact very closely interrelated.

TSPA Development and Analyses. At the same time as the abstraction activities are being completed, development of the architecture of the total-system software will be finished. In mid-November, 1997 through January 30, 1998, the base case will be run to assess the reference design and the nominal site models.

Upon completion of the base case, guidance will be given to the various abstraction groups concerning the construction of appropriate sensitivity analyses. In addition, TSPA models will be developed and implemented to assess the influence of disturbances to the nominal case (such as volcanism, seismicity, human intrusion, and nuclear criticality). TSPA models to represent additions or enhancements to the reference design will also be constructed at this time. Final TSPA analyses are scheduled to be conducted by June 1, 1998.

TSPA Status and Documentation. Results and preliminary interpretation of the base-case analyses are scheduled to be presented internally on January 30, 1998. A status of the additions to the base case are to be presented internally in mid-April, 1998, concurrent with the presentation of the sensitivity analyses and results for the abstractions.

Documentation of the TSPA base-case analyses and results of all sensitivity studies, and of final parameter sets, assumptions, rationales, results, and interpretations and conclusions are scheduled to be completed for the Draft TSPA-VA by June 12, 1998. This draft will incorporate the preliminary chapters described above, all revisions due to interim review comments, and discussions of the sensitivity analyses run for each component. The Draft TSPA-VA is to be reviewed by the DOE and other parts of the M&O between June 12 and July 15, 1998. Comment resolution is scheduled to be completed and the final TSPA-VA document will be submitted to DOE by August 20, 1998.

2.3 IMPORTANCE OF THE TSPA-VA

The YMP Performance Assessment (PA) organization is cognizant of the high visibility of the TSPA-VA both within and external to the Yucca Mountain Project. Several organizations will review and comment on the TSPA-VA. The expectations from two key groups, the U.S. Nuclear Regulatory Commission (NRC) and the Nuclear Waste Technical Review Board (NWTRB) are summarized below.

> NRC. The NRC has noted that the performance assessment to be described in TSPA-VA is the centerpiece of the DOE VA and ultimately the license application (Federline et al, 1996). NRC also notes that the DOE VA is not a regulatory document, but it will be the basis for decisions about the future of the national program for storage and disposal of HLW and spent fuel" (Federline et al., 1996; Sagar, 1997, p. 1-7).
>
> NWTRB. The NWTRB has noted that this iteration of TSPA "will play a different and clearly more prominent role than in the past" (NWTRB, 1997, p 21). The NWTRB also notes that "DOE's intention is for the TSPA-VA, its revisions, or successive iterations to play dominant roles in assessing compliance with the DOE's revised siting guidelines in 10 CFR Part 960 (currently scheduled for June 1999), recommending the site to the President (currently scheduled for 2001), and applying to the NRC for a license to construct the repository (currently scheduled for March 2002)" (NWTRB, 1997, p 21). Because of this, they observe that the "*absolute* level of the calculated risks" has increased importance, thus "placing additional burdens on the TSPA and requiring answers to two general questions:
>
> 1. Does the TSPA demonstrate the safety of the repository?
> 2. Does the TSPA generate confidence?" (NWTRB, 1997, p 21).

Clearly, the TSPA-VA is very significant to these groups. PA staff realize that the TSPA-VA document produced will elicit comments from a broad spectrum of concerned citizens. As a result of the intense scrutiny expected, support has been solicited from across the M&O organization to ensure that the TSPA-VA product will adequately support the viability assessment. PA is actively soliciting comments from the major review agencies through participation in internal integration meetings and public technical exchanges. The review agencies include the U.S. NRC, NWTRB, and TSPA Peer Review team, as well as various expert panels convened by the M&O to review the YMP process models and parameters. YMP has engaged the support of an external Peer Review Panel to evaluate the technical adequacy of the assumptions made in the TSPA-VA. PA has also initiated self assessments of some component modules of the TSPA to evaluate the traceability of the logic used to identify and prioritize key issues to be evaluated in TSPA-VA. PA will continue to monitor internal progress to produce a product that will meet the above expectations.

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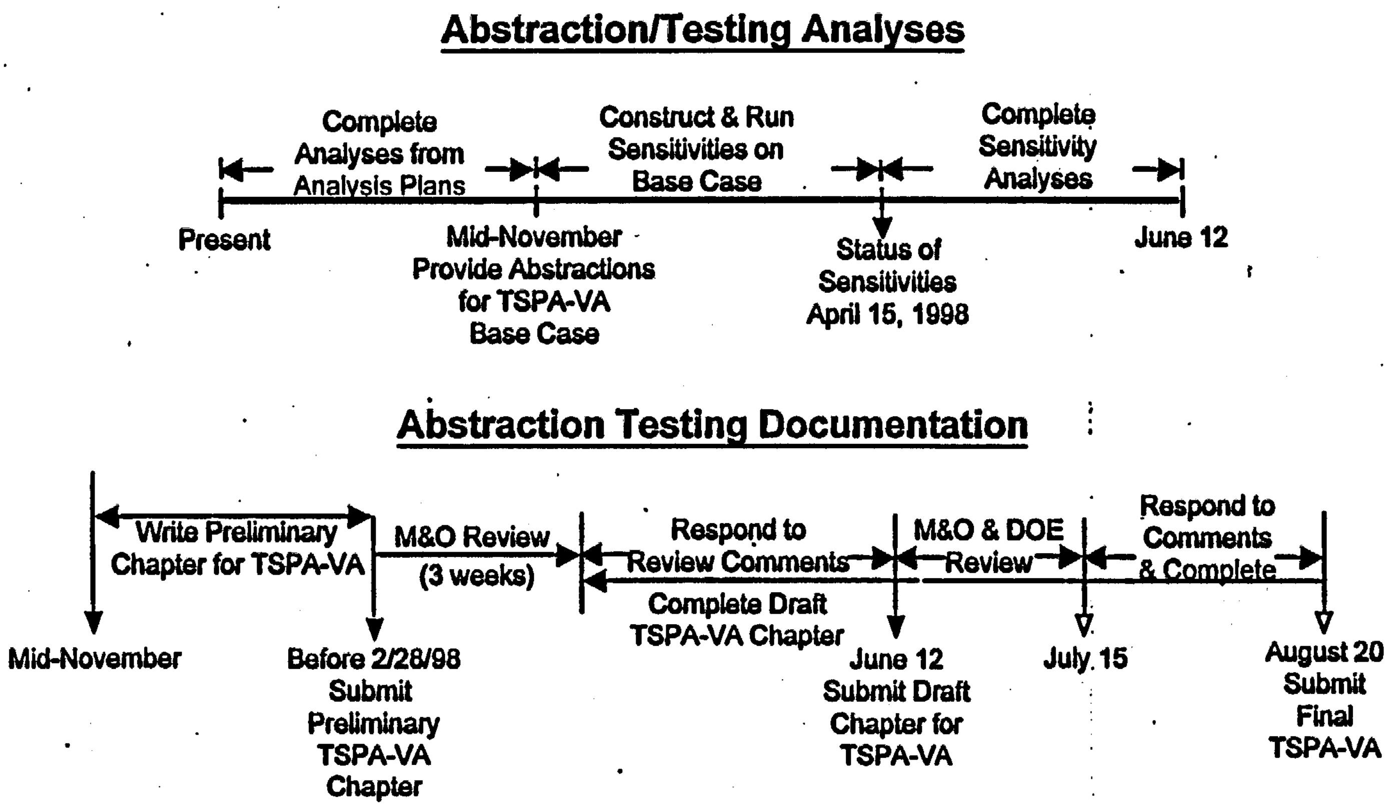

Figure 2.3-1. Schedule for Abstraction/Testing Activities Analyses and Documentation

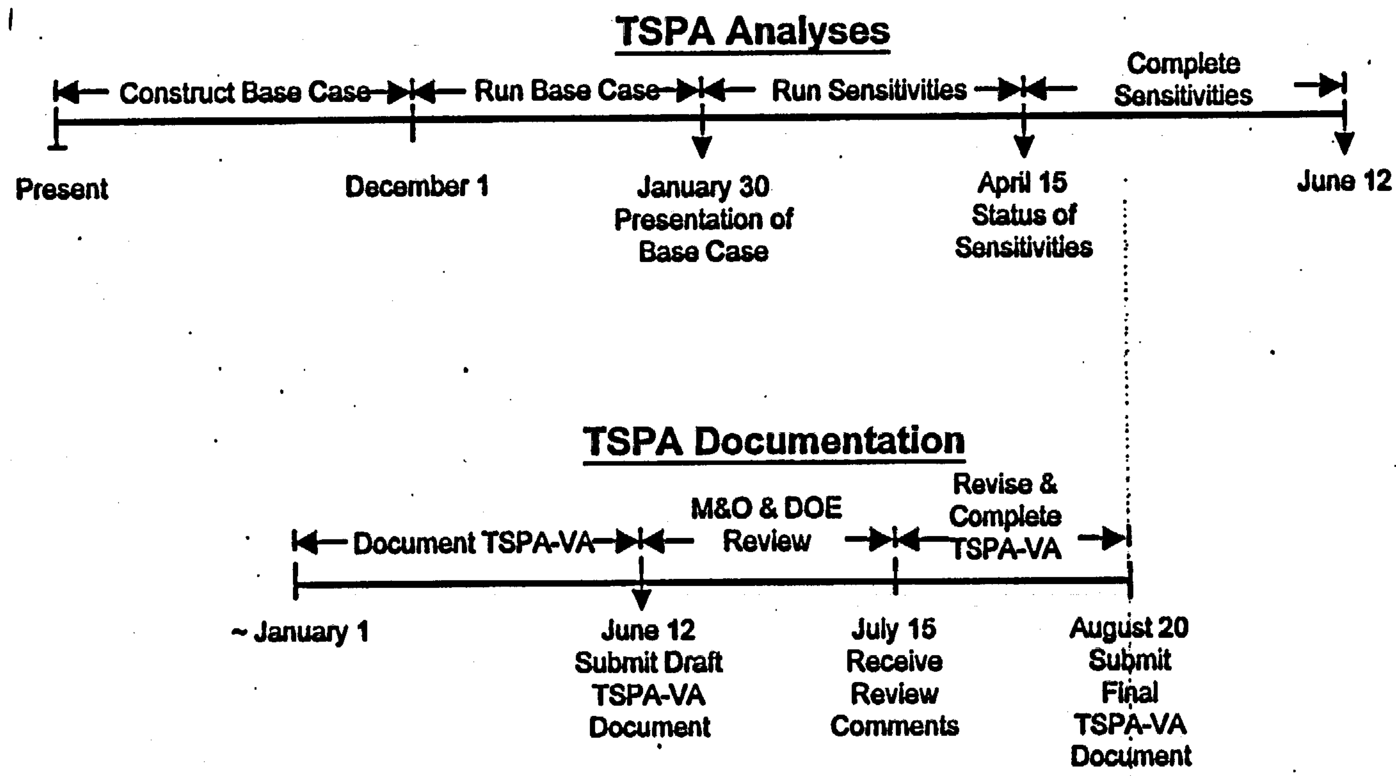

Figure 2.3-2. Schedule for TSPA Analyses and Documentation

3.0 HISTORY OF YMP PERFORMANCE ASSESSMENT ACTIVITIES

Holly A. Dockery, Ralston W. Barnard

3.1 OVERVIEW

Total System Performance Assessment, as defined in Chapter 2, is an analysis process in which important features, events, and processes (FEPs) of the waste containment and isolation system are represented in models of varying complexity to evaluate the behavior of the system against specified performance measures. A number of complete TSPAs (Sinnock et al., 1984; Barnard and Dockery, 1991; Barnard, et al., 1992; Eslinger, et al., 1993; Wilson, et al., 1994; Andrews, et al., 1994; and M&O, 1995) have been performed for the potential repository system at Yucca Mountain. In addition, several subsystem analyses have been performed. As more information about the site and design components of the potential repository system has become available, these TSPA analyses evolved into progressively more complex representations of the system.

The representation of some of the elements of the total system analysis included in each of the iterations has remained fundamentally the same, although the models and parameters have been revised and refined each time. However, as our understanding of the FEPs present in the system has progressed, the representation of certain process areas has been significantly updated. Perhaps the largest change has occurred in the understanding of unsaturated-zone groundwater flow at the potential repository site. Clearly, the rate and distribution of the movement of groundwater through the unsaturated zone is important to the performance of the system. In every TSPA, regardless of the details of the performance measure used, performance is highly correlated to unsaturated zone flow. In earlier assessments of Yucca Mountain, groundwater was assumed to flow downward, almost exclusively in the matrix. This assumption resulted in extremely slow flow through the entire system, and thus to very low cumulative releases during the regulatory period. Sensitivity studies at higher fluxes suggested it to be an important parameter. The evolution of the understanding of unsaturated-zone groundwater flow has required changes in our models and representation of the system. The most current model for this process is described in detail in Chapter 4 and in Section 6.1.

In addition, the design has been evolving in response to experimental data and a changing understanding of site characteristics. In particular, TSPA analyses have been required to change from representation of a small, in-floor, vertically emplaced waste package, as specified in the SCP, to a significantly larger waste package emplaced horizontally in the drift. For a postclosure TSPA, this change has required inclusion of analyses concerning 1) drift stability with time; 2) performance effects of backfill, pedestals, and invert materials; 3) amount and location of seepage into the drift; 4) lifetime of alternative container materials; and 5) possibility of single or common mode failures of multiple waste packages due to circumstances in the drift. Another large change in the design has been establishment of a high temperature region, utilizing the thermal output of the large waste packages. In an attempt to form a long-lived "dry-out zone" from the heat of the packages, and thus to extend package lifetimes by curtailing corrosion from inflowing groundwater, areal power densities of up to 114 kW/acre have been studied. The change to higher thermal load and larger waste packages, as well as other design changes related to use of concrete drift liners, drip shields, etc., have all required accommodation by the TSPA models.

Changes in regulatory guidelines have also resulted in major changes in the TSPA modeling activities. For instance, TSPA analyses that assessed the release of gaseous ^{14}C against the guidelines in 10 CFR Part 60 and 10 CFR Part 960 showed that this process provided the major contribution to the TSPA results when expressed in terms of cumulative releases over 10,000 years. However, the upper limit on releases of ^{14}C in these standards are far below annual release limits established by the Clean Air Act. If the new regulations, when repromulgated, are consistent with the Clean Air Act, ^{14}C is no longer expected to contribute significantly to the TSPA results. Another major change in TSPA models has resulted from conversion to a dose standard, resulting in increased significance of the saturated-zone flow. When the performance standard only addressed cumulative release, details of saturated-zone flow (e.g., dispersion, dilution) were relatively unimportant. Under a dose standard however, radionuclide transport through the saturated zone is very important. Thus, TSPA models and analyses have changed to reflect these and other changes required by the dose standard that is expected to be promulgated by the Environmental Protection Agency in response to the Energy Policy Act of 1992 (see section 2.1.2).

3.2 PRECURSORS TO RECENT YMP TSPA MODELING ACTIVITIES

One early study of the Yucca Mountain repository system utilized deterministic calculations of radionuclide release from the system using a one-dimensional transport code (Sinnock et al., 1984). This study also included some additional analyses to estimate the importance of the effects of dimensionality, particularly in terms of lateral diversion of unsaturated flow. This study considered primarily "nominal conditions", based on the then current site knowledge. However, it also assessed the effects of increasing groundwater flux up to 20 mm/yr and of decreasing radionuclide retardation (due to interaction with the rock minerals) to zero. The releases calculated along the groundwater pathways under nominal conditions were more than seven orders of magnitude below the EPA release limits. Uncertainties were not explicitly included in the TSPA, nor were gaseous releases. The authors recognized that both incorporation of fast-path flow and changes in the assumptions about fracture-matrix interactions, as well as different treatment of geochemical retardation and of the source term could have major implications in terms of meeting the standard then applicable (EPA 1995). No disruptive processes or events were included in this calculation. Analyses performed for the Environmental Assessment (DOE, 1986) evaluating the postclosure system guideline also concluded that releases, even over a period of 100,000 years would not exceed the EPA's 10,000 year release guideline. However, it was recognized that a great deal of uncertainty remained in the representation of the groundwater flow system and in the performance of the engineered system in oxidizing conditions in the unsaturated zone.

A number of subsystem analyses were performed in the subsequent years, including initial assessment of disturbances such as volcanism and human intrusion (Sinnock, 1989; Doctor et al., 1992, reporting 1988 work), waste package lifetime (Farmer and McCright, 1989), and performance of spent fuel (Apted, 1989). However, the predecessors to the current set of iterative performance assessments were the Performance Assessment Calculational Exercise (PACE-90) conducted in 1989 and 1990 (Barnard and Dockery, 1991) and the initial total systems analyses (Doctor et al., 1992, reporting 1988 work). PACE-90 was defined to simulate nominal-case groundwater flow and transport over a modeling period of 100,000 years. Deterministic analyses were run in both one- and two- dimensions. Four radionuclides were used to represent classes of behavior of long-lived nuclides present in the inventory (^{237}Np, ^{99}Tc, ^{129}I, and ^{135}Cs). Percolation flux through the repository horizon was set at 0.01 mm/yr . Waste was mobilized from two major water-contact modes: "wet-drip" and "moist-continuous". The nuclides then traveled through a 19-layer hydrostratigraphy with laterally homogeneous properties that was developed from limited information from four boreholes. There were no calculated releases to the water table during the specified time period, therefore movement in the saturated zone was not included. Also, gaseous releases, thermal effects, and disturbed scenarios were not included. The key aspects of this and the following TSPAs are summarized in Table 3-1.

3.3 TSPA-1991

The first in the "modern" TSPA studies conducted by YMP was TSPA-1991 (Barnard, et al., 1992; Eslinger, et al., 1993) constructed using PACE-90 as a basis. Its objective was to develop a framework for probabilistic total-system calculations and it was the first set of stochastic analyses for YMP. The analyses were run in one- and two-dimensions using distributions of hydrogeologic parameters based on site and analog data. Two conceptual models for UZ flow were analyzed: composite porosity that represented fracture-matrix equilibrium, and the "weeps" model that assumed flow occurred exclusively in the fractures. The calculations also included disturbances to the nominal system caused by basaltic volcanism, human intrusion, and climate change. The radionuclide inventory was expanded to include those nuclides prevalent in the inventory (Pu, U, and Am isotopes), those expected to be important to dose (^{79}Se, ^{126}Sn), and ^{14}C to represent the gaseous component. Radionuclide transport from the waste package also included some near-field interactions. The saturated zone was also included explicitly and modeled out to the accessible-environment (5 kilometers). A simple drinking water dose was calculated, in addition to the cumulative releases.

No attempt was made to evaluate regulatory compliance. Qualitatively, however, comparisons were made. Results for TSPA-91 suggested that aqueous releases for both the weeps and composite porosity models and gaseous release using the weeps model did not exceed the EPA standard's (EPA 1985) cumulative release limits. Gaseous release, calculated with the composite porosity model did exceed these limits. However it was anticipated that a more realistic EBS model for waste package and waste form failure (i.e., taking credit for gradual degradation of these engineered components) would reduce these releases to below the EPA limit. Releases due to human intrusion and to volcanism were also both well below these regulatory limits.

3.4 TSPA-1993

The primary purpose of TSPA-1993 (Wilson, et al., 1994; Andrews, et al., 1994) was to provide feedback concerning the relative importance of specific site-characterization and design information. Its secondary goal was to make progress in developing more defensible TSPA models for use in a demonstration of compliance.

There were a number of enhancements and revisions of the TSPA-1991 models and information including: a more geohydrologically representative model of the repository, a 3-D geostatistically correlated stratigraphy, an expanded hydrologic data set, explicit inclusion of wetter future climates, discrete modeling of individual geologic stratigraphy in the SZ, modification of retardation and sorption parameters, introduction of thermal dependence, spatial and temporal variation in fracture apertures (in the Weeps model), inclusion of waste-package failure modes due to corrosion and dry oxidation, updated waste-form dissolution and oxidation models, analysis of both the SCP containers and the MPCs, and inclusion of spent fuel and vitrified waste.

The analyses investigated sensitivities using both cumulative releases and dose results for up to 1,000,000 years. Percolation flux was the single most sensitive parameter. Again, as in TSPA-1991, all releases were below the EPA's 1985 standard, except for gaseous ^{14}C releases. However, longer-term (>100,000 years) peak doses for drinking water pathways were shown to be significantly above background. These analyses were being performed prior to the remanding of the EPA's 1985 standard (see section 1.1.2), and were not designed to evaluate regulatory compliance.

3.5 TSPA-1995

The objectives of TSPA-1995 (M&O, 1995) were primarily to enhance the representation of the engineered system, although some improvements of the natural system models were also incorporated.

Specific changes to TSPA-1993 models included: inclusion of a drift-scale thermohydrologic environment to derive relative humidity and temperature information adjacent to the waste package; a more detailed waste-package-degradation model, including corrosion of both inner and outer waste-package layers and galvanic protection of the inner layer; calculation of releases both with and without backfill; modification of solubility and retardation values for radionuclide transport; and consideration of two alternative ranges of percolation flux (high flux: 0.5-2.0 mm/yr; low flux: 0.01 - 0.05 mm/yr). Disruptive events and gaseous releases were not included in TSPA-1995. A simple climate-change model was also incorporated into the analyses. The time period for the calculation of release and dose was up to 1,000,000 years.

TSPA-1995 also reported percolation flux to be the single most important factor to performance of a Yucca Mountain repository in the context of a 10,000 year standard. However, many elements of the EBS also were key to performance, as shown through sensitivity analyses such as galvanic protection, varying thermal load and backfill configurations, and assumptions about radionuclide transport through the EBS. As in TSPA-1993, sensitivities were calculated in terms of system-level performance measures such as dose and cumulative release, and no attempt was made at evaluating regulatory compliance.

3.6 OTHER RECENT YUCCA MOUNTAIN TSPAs

A number of other organizations have performed TSPAs for Yucca Mountain in the past several years. The most recent iterations include TSPAs run by the NRC (NUREG-1464) and by the Electric Power Research Institute (EPRI) (Kessler and McGuire, 1996). A TSPA was also conducted by Sandia National Laboratories (Rechard, 1995) on a hypothetical "Yucca Mountain-like" tuff site. The suite of scenarios analyzed by each of these groups was essentially the same as those used in the YMP TSPAs. In each case, assumptions about conceptual models and parameter distributions differed somewhat from those of the YMP TSPAs. However, the conclusions reached about the importance of particular processes and parameters (with the possible exception of basaltic volcanism in the case of the NRC) in terms of performance of the repository system were essentially the same as those of the YMP TSPA analyses.

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Table 3.1-1. Analysis Approach to Selected Previous TSPA Evaluations

Feature	Sinnock et al, 1984	PACE-90	TSPA-91	TSPA-93	TSPA-95
Infiltration	up to 20 mm/yr	Min: .01 mm/yr Max: 0.5 mm/yr	0 – 39 mm/yr	dry: 0.5 mm/yr mean wet: 10 mm/yr mean	lo: 0.01-0.05 mm/yr hi: 0.5-2.0 mm/yr
# of Radionuclides	17	4	10	43 (direct) 8 (aqueous)	39
Time Period of evaluation	up to 100,000 yrs	up to 100,000 yrs	up to 100,000 yrs	up to 1,000,000 yrs	up to 1,000,000 yrs
Waste Forms	CSNF	CSNF	CSNF	CSNF and HLW	CSNF and HLW
Distance to AE	5 km	n/a	5 km	5 km	5 km 30 km
Saturated Zone	yes	n/a	single composite medium	multiple layers	single composite medium
Stratigraphic Discretization	n/a	19 layers	5 layers	10 layers	5 layers
UZ flow model	1-D, matrix	1-,2-D 5 codes	1-,2-D; ECM and Weeps	1-,2-D; ECM and Weeps	2-D; ECM
Release Model	n/a	2 water contact modes	simple failure distribution for WP	simple failure distribution for WP	3 alternative conceptual models in EBS

Table 3.1-1. Analysis Approach to Selected Previous TSPA Evaluations (continued)

Feature	Sinnock et al, 1984	PACE-90	TSPA-91	TSPA-93	TSPA-95
^{14}C gaseous release	no	no	2-D steady state	2-D transient	no
Thermal effects	no	no	no	dry-out zone	dry-out zone
Disruptive Events	no	no	volcanism, human intrusion	volcanism, human intrusion	no
Fracture Flow	no	in ECM	ECM, weeps	ECM, weeps	yes
Dose	no	no	no	Drinking water and irrigation	Drinking water
Climate Change	through range of fluxes	no	through range of fluxes	100,000-year random periods	100,000-year cycles
Galvanic Protection	no	no	no	no	yes
Uncertainty	through range of analysis parameters	no	in pdf's and flow models	in pdf's and flow models	in pdf's and flow models

Notes:
CSNF = commercial spent nuclear fuel
HLW = high-level waste
ECM = equivalent continuum model
Weeps = unsaturated flow model assumes stochastic flowing fractures
WP = waste package
EBS = engineered barrier system
pdf = probability distribution function

4.0 COMPONENTS OF TSPA

Robert W. Andrews, S. David Sevougian

An assessment of the total system performance of a repository system must consider all relevant features, events and processes (hereafter referred to as FEPs) that could significantly affect the containment and isolation of the radioactive materials from the biosphere. Although a wide range of potentially significant FEPs might be included in a total system performance assessment, the philosophy is to concentrate on those FEPs that are either (1) expected to occur over the design life of the repository with high probability or (2) have a low probability of occurring but have potentially significant consequences to human health and the environment if they occur. The objective of the performance assessment is to evaluate the possible consequences of all potentially significant FEPs in order that informed decisions can be made regarding the risks associated with different design alternatives.

It has been common practice to break the overall system into individual components that can be separately described and modeled. In general one may consider the system being comprised of six major elements that must be evaluated: (1) the natural environment unperturbed by the presence of underground openings or emplaced wastes, (2) the perturbations in the natural system caused by the construction of the underground facilities and the emplacement of wastes, (3) the long-term degradation of the engineered components designed to contain the radioactive wastes, (4) the slow release of the radionuclides from the engineered containment system, (5) the migration of these radionuclides through the engineered and natural barriers to the biosphere, and finally (6) the ultimate uptake of these radionuclides by plants, animals and humans leading to a dose consequence.

Prior to describing *how* a total system performance assessment is performed (Chapters 5, 6, and 7), it is useful to discuss *what* is being analyzed. The definition of *what* is being analyzed should be preceded by a description of *how* the repository system is intended to function and the processes that need to be incorporated in the analyses.[1] In the following paragraphs (Section 4.1) we first present a sketch of *how* the repository system is intended to work, including a description of the base case design and design options. Following that discussion, we describe in Sections 4.2 and 4.3 *what* processes are being modeled to develop the quantitative description of *how* the repository will behave. In Chapter 5 we give an overview of *how* the TSPA-VA will be performed. In Chapter 6 we present the details of *how* the process models are being abstracted for TSPA-VA. In Chapter 7

[1] The notion of presenting *what* is being analyzed, including a description of *how* the repository system is intended to work, before presenting *how* the system is being analyzed was a recommendation provided in the First Interim Report of the Total System Performance Assessment Peer Review Panel (Whipple et al., 1997, p 10). In the Panel's view, it was felt that a key aspect of achieving traceability and transparency in a TSPA analysis is to first communicate the overall description of the repository system and the processes to be modeled so that the reviewer understands what is being analyzed prior to discussing the details of how it is analyzed. We agree with this recommendation and have provided some preliminary text that we hope elucidates the intended functions and processes that impact long term waste containment and isolation at Yucca Mountain.

we present the details of *how* the abstracted models are being used in TSPA-VA. In summary, in this chapter we will present a discussion of *how* the repository system is intended to work and the components that need to be analyzed, and in subsequent chapters we will present *how* we intend to analyze these processes and their impact on total system performance.

4.1 *HOW* THE YUCCA MOUNTAIN REPOSITORY SYSTEM IS INTENDED TO WORK

General descriptions of how deep geologic repository systems are intended to contain and isolate radioactive wastes from human contact are available in several recently published articles in a Special Issue of *Physics Today* on Radioactive Waste (Ahearne, 1997; Crowley, 1997; Kastenburg and Gratton, 1997; North, 1997; and McCombie, 1997). However, it is informative to walk the reader through the details of how the Yucca Mountain repository system in particular is intended to work to meet the objectives of isolating the wastes for a sufficiently long time period that the natural decay of the key radionuclides will reduce the risks of human exposure to acceptably low levels.

One could either start this discussion from the perspective of the radioactive wastes and look progressively outward through the multiple barriers (both engineering and natural) that are intended to contain and isolate the waste or, conversely, we could start from the perspective of the individuals and populations that the repository barriers are meant to protect from the potentially harmful effects of radioactive wastes and look progressively inward through the multiple barriers. We have chosen the former route.

The following discussion is meant to focus on the performance assessment related attributes of the waste disposal system, attributes that need to be evaluated and ultimately quantified in making predictions of the evolution of the system and the consequences associated with disposing radioactive wastes at Yucca Mountain. Other discussions of the system components from the perspective of repository design and the concept of operations are documented in M&O (1997a). Additional presentation of these components from the perspective of communicating the strategy for demonstrating acceptable levels of safety are documented in the Waste Containment and Isolation Strategy (DOE, 1996 and M&O, in preparation).

In order to assist the reader in following the discussion of how the repository system is intended to work, the basic elements of the system as well as the reference design are described. Figure 4.1-1 schematically illustrates the basic elements of the site and engineered barriers that affect the predicted behavior of the system. The figure shows the key characteristics and components of the total system, with an expanded look at the engineered barrier system (EBS).

4.1.1 Reference Design

The base case design for TSPA-VA analyses is expected to be completed in September, 1997, the so-called "Reference Design". We will refer to this design as the base case design for TSPA-VA. The basis for the base case design is presented in this section. Much of the text was extracted from

M&O (1997b). The design has been formulated with the intention of enhancing system performance with respect to the key system attributes described in the WCIS (DOE, 1996), including 1) rate of water seepage into the repository, 2) waste package lifetime (containment), 3) rate of release of radionuclides (mobilization) from breached waste packages, 4) radionuclide transport through engineered and natural barriers, and 5) dilution in the saturated zone below the repository. The design strategy seeks to use engineered components to tailor the environmental variables (i.e., temperature, relative humidity, seepage flux) to be as benign as possible.

A schematic of the base case design at the time of repository closure is presented in Figure 4.1-1. In general, the major components of the base case design will include a high areal mass load (85 MTU/acre), with "point loading" of the waste packages. The engineered barrier system will include a drift liner (concrete), an initial air gap in the drift (no backfill), two-layer waste package [(10 cm corrosion allowance material (CAM) and 2 cm corrosion resistant material (CRM)], in-drift emplacement of the waste packages, placement of the waste packages on a steel pedestal, and a concrete invert at the base of the drift. The following discussion provides more detail as to the basis for each of these design components.

Drift Liner (Normal Concrete). A drift liner has been included in the design, primarily in support of pre-closure safety. While it is intact, the liner is a potential barrier to seeping water, which has the opportunity to drain through the small space between the liner and the host rock and also to film-flow along the inside surface of the liner. Both of these modes of flow reduce or eliminate dripping directly onto the WP. Normal concrete is used in the current reference design.

Air Gap (Capillary Barrier). The air gap between the liner or drift wall and the waste packages, provides a means by which percolation flux may be diverted around the opening as matrix or film flow. This advantageous property will be in effect until the drift collapses and fills with rubble.

Waste Package - Corrosion Allowance Material (CAM). Because the waste package is the single component that is expected to have absolute containment at the time of emplacement, the design strategy is to make the waste package robust. The outer layer of the WP, the CAM, is 10 cm thick and serves three functions. First, it provides structural strength to resist rockfalls, to support the internal components, to be supported by the pedestals, and to be handled. Second, the CAM provides radiation shielding to reduce the WP exterior surface contact dose rate. Coupled with the MGDS transport overpack, the shielding is enough to protect workers. Third, the CAM acts as a containment barrier for the radioactive waste inside the WP. The current CAM material in the design is a carbon steel, Alloy A516.

Waste Package - Corrosion Resistant Material (CRM). The inner layer of the WP is a nickel based alloy that is very resistant to aqueous corrosion and nearly totally resistant to humid air corrosion. The current reference CRM is 2 cm of Alloy 625. Because the CRM is inside the CAM, the corrosion environment can be much different than the ambient seepage water (potentially higher pH and crevice corrosion), thus requiring a more corrosion resistant material than the outer barrier.

Large Waste Packages. A large waste package reduces cost, handling, closure operations, non-destructive evaluation (NDE) operations, and allows efficient use of the drift length. The current large waste package reference design is based on a 21 PWR Spent Nuclear Fuel (SNF) Assembly WP. Roughly the same size WP can also accommodate 44 of the smaller BWR SNF Assemblies or five Defense High Level Waste (DHLW) glass "logs" surrounding a central canister of DOE SNF. For high heat producing, or high criticality potential, assemblies, a smaller WP, for 12 PWR SNF Assemblies, is used.

In-drift Emplacement of Waste Packages. The design calls for in-drift emplacement. This is a consequence of large WPs being well suited to in-drift emplacement; consequently, the amount of excavation is minimized. Non-drift emplacement would require additional excavation.

Invert. The invert is designed to provide support for the WP pedestals during the preclosure period. It will be composed of normal concrete.

Pedestals. The carbon steel pedestals provide support for the WPs during the preclosure period. The pedestals will be installed at a pre-determined spacing such that each WP is guaranteed to have at least three pedestals under it, independent of WP spacing.

Thermal Design - Areal Mass Load (High). The areal mass load (AML) for the base case is 85 MTU/acre. This was determined by consideration of cost, and expectation of water driven away during the high temperature period, and preservation of the zeolites below the repository. Clearly, if performance were independent of AML, it would be most cost effective to load the waste as densely as possible (high AML). Thus, the goal is to load the repository at as high an AML as feasible for acceptable performance, in order to minimize cost. In May 1995, the OCRWM Director decided to focus on a reference AML range of 80-100 MTU/acre, while maintaining the flexibility to use alternate AMLs should performance calculations find the reference range to be unacceptable. The current reference design AML is set by the temperature maximum which won't degrade the zeolites (potential radionuclide transport retardation mineral) below the repository.

Thermal Design - WP Spacing (Point). Once an AML is determined, the designer has the option to emplace closely spaced WPs in widely spaced drifts or to emplace the WPs farther apart in less-widely-spaced drifts. The latter option is termed "point loading" because each WP acts relatively independently of its neighbors in shedding its heat (this independence is strongest at very early times, before the rock heats up between the WPs). Of course, there is a considerable range of combinations of WP spacing and drift spacing that meets this definition of "point". The current reference design has a drift spacing of 28 m. The current drift spacing of 28 m is set by a 200°C limit on the drift wall temperature.

Thermal Design - SNF Assembly Blending - To Meet 18 kW Limit. Each SNF assembly has a specific set of characteristics: Enrichment, burnup, and age. These determine how much thermal power the assembly produces. A limit of 18 kW has been set for the collection of assemblies in a WP to prevent heating the cladding beyond 350°C, which could cause it to perforate. For the 18 kW "Design Basis" WP at a drift spacing of 28 m, enough aluminum is used in the basket design to ensure the cladding does not exceed the temperature limit. SNF assemblies will be packaged appropriately to meet the 18 kW limit.

Thermal Design - SNF Assembly Blending - To Meet Criticality Limit. Each SNF assembly also has a specific potential to contribute to nuclear criticality, again based on enrichment, burnup, and age. This potential is quantified by the criticality constant in an infinite lattice, k_∞. Based on the finite number of assemblies in the WP and the overall effective criticality constant constraint, $k_{eff} < 0.95$, limits have been set for assembly values of k_∞. SNF assemblies will be packaged to meet limit.

Design Option Sensitivity Cases.

The VA Design is expected to include the aforementioned base case design as well as several design "options". The highest priority options currently being investigated (M&O, 1997b) are: 1) ceramic coatings on the waste packages, 2) ceramic "drip shields" supported by the waste packages, and 3) backfilled emplacement drifts. Backfill is not regarded as one of the highest-priority options on its own, but only in combination with ceramic coatings or drip shields, primarily intended as protection to the ceramics from rockfall. Another item that is sometimes mentioned as a design option is "cladding credit," i.e., taking credit in the performance assessment for potential protection of spent fuel by its cladding (Zircaloy, in most cases). While not really a design option, including or not including cladding credit in the TSPA calculations will be a type of sensitivity analysis for TSPA-VA. Figure 4.1-2 indicates the location of these design options. The basis for consideration of these design options is summarized below. Again, much of the discussion on the alternative design options is extracted from M&O (1997b).

Ceramic Coating (on the Outside of the WP). Ceramics have the advantage of being thermodynamically stable; they are the end-point of oxidation. Natural analogs of ceramics are millions of years old, and some of the oldest human artifacts (tens of thousands of years old) are ceramics. Thus, it is expected that a ceramic component on the WP could provide defense in depth by protecting the other WP materials from corrosion due to moisture. For a ceramic to perform this function, it must 1) cover the entire WP without any cracks or unsealed seams, 2) have sufficient thickness to essentially eliminate diffusion of water, 3) have sufficient density (of low porosity and permeability) so that water cannot penetrate it, and 4) remain intact. The ceramic must also be protected from other mechanical loads (e.g., falling off a degraded pedestal, seismic loads, and loads due to the mass of the collapsed drift on the WP at later time). Fabrication of a coating on the WP substrate is much more feasible than construction of large stand-alone ceramic shells. Candidate materials for ceramic coatings are Al_2O_3 (alumina), TiO_2 (titania), $MgAl_2O_4$ (spinel), and ZrO_2 (zirconia).

Drip Shield - Supported by the WP. Corrosion of the WP is enhanced by the presence of liquid water (high humidity also can cause corrosion). Furthermore, liquid water is required to mobilize and transport most radionuclides. In addition, the site characterization organization has concluded that percolation flux at the repository horizon is primarily in fractures with a small part of that fracture flow being episodic. Near the surface, there have only been eight detectable infiltration events during the last four years; this is episodic. At repository depth, there is evidence which suggests episodic percolation. Where active flowing fractures couple with sharp drift wall edges, seeps (drips) into the drift can occur. It is the function of the drip shield to divert these drips from the WP. (The possibility of condensation between the WP and the drip shield cannot be ignored, however, so the drip shield prevents much, but not all of the possible water contact.) If the diverted seepage flux is drained without passing through the part of the invert contaminated by the radionuclides from failed WPs, diffusive transport will pertain in the EBS, and dose rates will be greatly reduced. Thus, part of the design of an effective drip shield is to physically separate the water that it sheds from water that condenses under it and flows through breached WPs. For VA, we are only considering a drip shield in the form of a cylinder or half cylinder surrounding or supported by the WP itself. A design analysis of this configuration is in review. As for the ceramic coating option, management has directed that backfill be included whenever drip shields are considered, since rock fall can degrade the performance of an otherwise long-lived ceramic or corrosion-resistant-metal drip shield. The constraints on ceramic coating mentioned above, apply to this component as well.

Backfill - Rock Fall Protection. The description of the two previous alternative design components includes scenarios in which the concrete liner and parts of the near-field rock fall into the drift. Covering the waste package with backfill protects other components from damage from such mechanical loads. A design analysis has shown that the waste package can withstand impacts from very large rocks; an uncorroded WP can withstand the fall of a 38 ton (3.2 m dia.) rock, a 50% corroded WP can withstand a 24 ton (2.7 m dia.) rock, and a 75% corroded WP can withstand a 3.5 ton (1.4 m dia.) rock. For ceramic coatings and drip shields, much smaller rocks can cause localized damage that can be later exacerbated by water contact, since corrosion of the substrate can cause expansion, peeling the coating. Therefore, management has directed that backfill be included whenever drip shields or ceramic coatings are considered.

Cladding Credit. The commercial radioactive waste is contained within a uranium dioxide matrix (fuel pellets) stacked in columns (fuel pins) which are clad in a sealed pressured Zircaloy tube (with walls about 0.6 mm thick). In reactor operation, the higher internal pressure due to operating temperature is balanced by the exterior coolant pressure. Less than 1% of the pins are expected to be perforated when the waste is accepted into the Waste Management System, and the Certificate of Compliance for the Regional Service Agencies is expected to document maintenance of that cladding quality. During the thermal period, cladding may fail if the cladding temperature exceeds 350°C for a substantial period of time, allowing creep to expand the tubes, thinning the cladding, and eventually allowing it to rupture (creep-rupture) and, the WP is breached before the temperature falls below about 200°C because above this temperature (the threshold is somewhere between 200 and 260°C). The SNF exposed by the perforation can quickly oxidize, and expand (opening the perforation further), until the cladding unzips along most of its length. If either event does not occur, some credit may be taken for cladding isolation of the waste. It is unknown how much the perforation of the cladding (either before waste acceptance or within the WP) will allow access to mobilize radionuclides at later times. For conservatism, it was agreed in the M&O Senior Management meeting (to review TSPA) on September 8, 1997, that only one order of magnitude credit should be taken for cladding performance.

The aforementioned design features have been included in an effort to provide a more robust EBS, which delays the degradation of the waste packages, leading to later, slower release from the EBS. With the exception of the backfill, very little information is available to support the evaluations of these design features. The performance of such features over long time periods is also uncertain. Nevertheless, in order to support the analysis of the design options, TSPA-VA will need to analyze at least the following design cases:

1. The reference design (which includes no ceramic coatings or drip shields, and no backfill) without cladding credit.

2. The reference design with some degree of cladding credit (the TSPA-VA "base case"), perhaps sampled probabilistically.

3. An alternative design in which waste packages are coated with ceramic (to provide additional protection against corrosion) and emplacement drifts are backfilled. (Backfill material has not been chosen yet. Tuff gravel and quartz sand are currently under consideration. Perhaps both would be analyzed, splitting this case into two cases.) Cladding credit included.

4. An alternative design in which waste packages are protected by ceramic drip shields (low-permeability ceramic designed to deflect water seeping into emplacement drifts away from waste packages) that are supported by the waste packages, and emplacement drifts are backfilled. (See comment above about backfill material.) Cladding credit included.

5. An alternative design that includes both ceramic waste-package coatings and WP-supported drip shields, plus backfill. Cladding credit included.

Additional design alternatives may be analyzed if time permits. Some alternatives of interest are: the use of alternative metals for the corrosion resistant materials, backfilled drifts without use of ceramic coatings or drip shields, "line loading" rather than "point loading" (that is, emplacing the waste packages very close together in order to equalize temperature and humidity between hotter and cooler packages), and use of additives in backfill or invert in order to manipulate the geochemical environment. In addition, disturbed scenarios may be analyzed in terms of potential common-mode failures, such as would be caused by a defective batch of waste packages, or a disruption affecting an entire drift-full of waste packages.

4.1.2 Description of Radioactive Wastes

The radioactive wastes to be disposed of at Yucca Mountain originate from neutron irradiation of uranium fuels in civilian and defense reactors. The major constituents of this waste consist of "unburned" uranium, actinide elements created by neutron capture and other reactions (such as curium, americium, plutonium and neptunium), and fission products. The radioactive constituents of nuclear wastes have varying decay rates and levels of toxicity and these wastes can remain toxic for very long time periods [see Figure 2 of Crowley, 1997]. Similar plots of toxicity versus time indicate that after a few tens of thousands of years, the radioactive wastes, though concentrated, have the same level of toxicity as the original uranium ore body had it been left in place [see Figures 2-3 to 2-5 in OTA (1985)].

The radioactive wastes to be disposed of are in the form of either spent nuclear fuel (from various sources including primarily civilian and defense reactors) or vitrified glass logs. The Nuclear Waste Policy Act allows for 70,000 metric tons of high-level wastes to be disposed of at Yucca Mountain, of which 63,000 metric tons are commercial spent nuclear fuel from civilian reactors and 7,000 metric tons are from defense reactors, including DOE spent fuels and Navy fuels, or vitrified glass. Spent nuclear fuel consists of the irradiated fuel itself surrounded by a thin corrosion-resistant Zircaloy cladding. The glass wastes consist of the glass matrix and an outer stainless-steel pour canister.

4.1.3 *How* the Engineered Barriers are Intended to Work

The objective of the waste disposal concept at Yucca Mountain is to keep the radioactive constituents contained within the waste form for as long a period as possible to permit the decay of a large portion of the radioactive material and to then limit the rate of release of the remaining radionuclides over a long time period. In order for the waste form to be altered and the radioactive constituents to be released to a mobile phase (predominantly water), the Zircaloy cladding (in the case of spent fuel) or stainless-steel pour canister (in the case of HLW glass) must first be breached. Although the spent fuel and glass waste forms can be altered in the presence of air, their dissolution rate, which controls the rate at which dissolved radionuclides are released to a mobile phase, is dependent on the availability of moisture. The dissolution rates may be on the order of thousands to tens of thousands of years depending on the moisture available for contact with the waste form. [As we will enumerate in the following discussion, the availability of moisture in both liquid and vapor form becomes the key driver in the overall performance of the Yucca Mountain repository system. Also, a useful summary of the key attributes of the waste disposal system can be illustrated by tracking how water moves through the various natural and engineered barriers, as presented below in Section 4.2.]

Prior to the breaching of the cladding or pour canister, it is necessary to first breach both the outer and inner layers of the waste package. The degradation modes and rates of the waste package materials are a function of the thermohydrologic and thermochemical environments on the waste package surface, the materials ultimately selected for the corrosion allowance outer layer and the corrosion resistant inner layer of the waste package, the degree of galvanic coupling between the outer and inner waste package metals, and the presence or absence of any additional materials placed on or over the waste package to delay the initiation of corrosion processes (such as the possible use of ceramic coatings, ceramic drip shields or backfill—see Figure 4.1-3). Note these additional materials are not included in the base case for TSPA-VA.

Once an initial opening through both layers of the waste package occurs, the environments outside and inside the waste package will generally equilibrate. A possible exception occurs with respect to any potential pendular (e.g., dripping) water, which may require a significant degree of waste-package degradation to penetrate the corrosion products built up on the outer surface of the waste package. While the waste package is intact (i.e., with no openings penetrating both layers), the radionuclides contained within the waste form are expected to remain within the waste form. Therefore the clock for potential releases from the waste form does not start until both the waste package and the cladding have been breached. This time period for breaching can range from thousands to tens or even hundreds of thousands of years. Once the clock has started, the waste package, cladding, and waste form all play a very significant role in controlling the rate at which radionuclides are released from the waste form and transported through the degraded waste package.

As noted above, a key aspect of the degradation of the engineered barriers (in particular the waste package, cladding, and waste form) is the environment in which these engineered components exist. The environmental conditions affecting these barriers include the thermal, hydrologic, mechanical, biological, and chemical conditions. These environmental factors are in turn a function of the design of the repository and waste-emplacement drifts (tunnels) (notably the thermal load resulting from emplacing waste, the underground support system used to assure retrievability during the operational phase, and the presence or absence of backfill in the drifts) and the *in-situ* ambient hydrogeochemical conditions (notably the thermal/mechanical/hydrologic characteristics of the host rock, the chemical conditions of the pore fluids and the local percolation flux through the host rock in the vicinity of the drifts).

In general, it is the hydrologic conditions in the drift that most significantly affect the degradation rate of the waste package, which dictates the desire to maintain as low a relative humidity for as long a time as possible on the waste package surface. In addition, it is the hydrologic conditions in the drift (in particular the amount and form of any seepage flux into the drift and the liquid saturation in any degraded materials between the waste form surface and the edge of the drift) that most significantly affect the potential releases from the engineered barriers once the waste package and cladding containment have been breached. One of the key attributes of waste disposal in unsaturated media such as at Yucca Mountain is that the amount of seepage into underground openings is a small fraction of the total flux. Because the capillary forces (within both the rock matrix and small fractures) that hold liquid water in the rock are generally significantly greater than the gravitational forces that allow pendular water to form, most of the percolation flux in the rock will continue around the underground drifts and not enter the drift. In local areas it is possible that the flux may be sufficiently high or the fracture characteristics such that dripping may occur. This flow into the drift may manifest itself as either film flow down the sides of the drift walls or as individual seeps. The phenomenon of capillary suction exceeding the gravitational forces required for seepage is expected to occur whether or not the drifts have collapsed as the capillary forces in the rock following collapse are still significantly greater than the large porous media in the collapsed drift.

4.1.4 *How* the Natural Barriers are Intended to Work

The hydrologic conditions in and around the drift are predicated on the hydrologic conditions in the host rock. The hydrologic conditions prior to repository construction and waste emplacement are generally controlled by downward, gravity-driven percolating water which infiltrates at the surface. The downward percolation flux is partitioned between a continuum that ranges from the micron-sized pores of the rock matrix up to millimeter-sized continuous fracture pathways. The average percolation flux, as well as its distribution in space and time, is not a measurable quantity but is derived from the unsaturated zone flow model, which is calibrated with a wide range of observed conditions, including matrix saturations and potentials, temperature profiles, chloride concentrations, ground-water isotopes such as carbon-14 and chlorine-36, pneumatic pressure response, and the presence of perched water bodies. The percolation flux is expected to change with time as a result of the thermal perturbation caused by the emplacement of the radioactive wastes (time period of hundreds to thousands of years) and the result of climate changes due to either anthropogenic effects (the greenhouse effect) or a return to pluvial conditions (time period of thousands to tens of thousands of years). These changes in the ambient hydrologic system need to be considered as the design life of the facility is for tens to hundreds of thousands of years.

Following the loss of containment of the waste package and the release of radionuclides from the engineered barriers, the dissolved and colloidal radionuclides will be transported in the ground-water within the unsaturated zone and saturated zone eventually to any potential receptors down gradient. Due to the sorptive capacity of the tuffaceous rock units along the likely flow paths, a significant fraction of the total mobilized and transportable radionuclides will be adsorbed on the mineral grains of the rock matrix and fracture surfaces or filtered out. Those radionuclides that are poorly adsorbed or not filtered in the case of colloids, may migrate through the unsaturated zone to the water table where they will mix with the lateral flow in the saturated zone. The distribution of arrival times of the different radionuclides at the water table surface will be a function of the percolation flux, the distribution of that flux between the fractures and matrix of the different lithologic units between the repository and the water table, any permeable fast pathways, the diffusion of radionuclides between the fracture and matrix media, the small scale heterogeneities of the velocity field within and between lithologic units (i.e., dispersion), the sorptive capacity of the lithologic units, and the release rate from the EBS.

Once the radionuclides are released from the unsaturated zone to the water table, they will ultimately mix with the flowing ground water in the saturated zone and be transported down gradient to potential receptors. The mixing with the significantly greater volumetric flux in the saturated zone will cause a reduction in the concentration of the dissolved radionuclides. Additional mechanisms that will tend to reduce the dissolved concentration include lateral and transverse dispersion caused by varying scales of velocity heterogeneity and the adsorption of radionuclides on the mineral surfaces.

Ultimately the ground water in the saturated zone will discharge to the surface, either at natural discharge locations (e.g., springs, seeps, or playas) or wells. In the Amargosa Valley, the bulk of the present discharge is to wells. The ground water extracted from these wells (or their equivalent in the future) may be used for irrigation, drinking water, and other domestic and commercial uses. Any radionuclides within the water that is extracted for public use has a chance of moving through various biosphere pathways and ultimately being ingested. Ingested radionuclides will lead to a dose to those populations exposed. Other exposure pathways include inhalation and direct exposure. The magnitude of this dose will be a function of all the processes we have enumerated above.

4.2. TRACKING WATER MOVEMENT THROUGH THE NATURAL AND ENGINEERED BARRIERS AT YUCCA MOUNTAIN AS A MEANS TO DEFINE THE KEY PROCESSES AFFECTING WASTE CONTAINMENT AND ISOLATION

Water is the principal medium by which the radioactive constituents in the waste form may be mobilized and transported to come into contact with the biosphere and ultimately humans. It is therefore instructive to examine the individual components of the waste disposal system in the context of the effects of water on these components. In the following discussion, we track water movement through the system from precipitation at the surface of the mountain to the groundwater used for human consumption or irrigation.

The following discussion consists of a series of conceptual models which, when properly linked, define the overall hydrologic system expected at Yucca Mountain. Although we recognize that alternative conceptual models exist (as discussed in the various sections of Chapter 6 related to hydrologic processes and their impact on post-closure performance), the discussion below continues the presentation of *how* the repository system is intended to work. The alternative models will be evaluated as part of TSPA-VA, as discussed in Chapter 7. Figure 4.2-1 presents a conceptualization of the flow through the natural and engineered barrier systems which can be referred to in this section concerning water movement through the system. Figure 4.2-2 presents a schematic of potential water flow into the EBS, both film flow and dripping water. The dripping water may flow into the waste package through a breach, or it may flow on the outside of the waste package. Ultimately, the water flow may exit the EBS at the base through the invert (see Figure 4.2-2).

4.2.1 Water Movement above the Repository Horizon

Precipitation in the Yucca Mountain region occurs as both rainfall events and snowmelt. Although a significant fraction of the precipitation over the potential repository either runs off to lower elevations or evaporates, some of the precipitation enters the soil or rock that is exposed at the ground surface. Some of this water that infiltrates the upper few meters of the soil horizon is lost to the atmosphere by either evaporation or transpiration through the roots of the native vegetation. The remaining water continues to migrate downward through the unsaturated (vadose) zone driven by gravity. This water is commonly referred to as the "infiltration flux," or at the repository horizon (i.e., elevation) as the "percolation flux."

Although some lateral diversion of the vertically percolating water can occur along interfaces between lithologic layers with different hydrogeologic properties, in general the water which escapes the evaporation/transpiration in the upper few meters of the soil horizon continues downward and will ultimately intersect the potential repository horizon. This downward percolating water is contained both within the rock matrix and the fractures of the different lithologic units. Generally, the welded tuff layers have a greater percentage of the total flux contained within the fractures (as the permeability of the matrix is low) while the non-welded units (in particular the Paintbrush above the potential repository horizon and the Calico Hills below the potential repository horizon) have a greater percentage of the total flux contained in the matrix (as the permeability of the matrix is high). Although designating the components of flux in the fractures and matrix is a useful way to describe the overall flow system, it should be remembered that a more or less complete spectrum of flow varying from the pores in the matrix through different scales of fractures (from microfractures of limited extent and aperture up to major fracture and fault networks that cut through entire lithologic layers) is expected to be present at Yucca Mountain.

4.2.2 Water Movement at the Repository Horizon

The ambient hydrology is expected to be perturbed by the presence of the underground openings and the subsequent emplacement of the heat-producing radioactive wastes. During construction and other phases of underground operations a significant amount of ventilation will be required. This ventilation will tend to dry out the rock matrix and a significant amount of water (primarily vapor) will be exhausted to the atmosphere.

Following waste emplacement, the heat generated by the waste will drive off moisture in the rock allowing it to recondense in cooler regions above, below, and between the emplacement drifts. During the first few hundred to few thousand years following waste emplacement and repository closure (the time period being dependent on the local thermal and hydrologic conditions and the design of the repository) the relative humidity in the drifts will be depressed and will slowly recover to the high ambient values (~99%). The liquid water in the rock will tend to stay in the rock due to the capillary forces in the rock pores and small fractures being greater than the gravitational forces. At some locations along the drift axes it is possible that local seeps of pendular water into the drift opening may occur once the above boiling conditions have subsided. In summary, the total volumetric water flux at the repository horizon will be distributed between a volume of flow around and between the drifts, a volume of flow into the drifts, and a vapor phase component in the drifts; and these will vary with time as the radioactive decay heat dissipates.

4.2.3 Water Movement in the Repository

The presence of water in both the vapor and potentially liquid phase in the drifts affects the long term degradation of the waste packages designed to contain the radioactive wastes. The current waste package design consists of two layers of metal, a 10-cm thick corrosion-allowance material (mild steel) and an inner 2-cm thick corrosion-resistant material (Alloy 625). As discussed in more detail in Chapters 6 and 7, alternative designs being considered include the use of alternative metals, a ceramic coating on the surface of the waste package, and a ceramic drip shield on top of the package to assure that any pendular water (i.e., drips) does not contact the waste package or waste form. The primary degradation mechanisms of the waste package are by aqueous or humid-air corrosion and possibly stress corrosion cracking. In the absence of any liquid water and in low (less than about 70%) relative humidities, the selected materials for the waste package are expected to last several tens to even hundreds of thousands of years. In the presence of humid air, the outer corrosion-allowance material will slowly corrode, eventually exposing the inner corrosion-resistant material. If ceramic coatings are placed on the waste package, it is believed that the initiation of humid-air corrosion can be delayed, extending the lifetime of the waste package. Once the outer metallic layer has been breached, the inner corrosion-resistant material will begin corroding, although there will be some time period during which the outer barrier may galvanically protect the inner metal. The degradation rate of the inner barrier also depends on the presence of liquid water on the surface as these metals show virtually no corrosion in humid-air environments. In summary, the degradation rate of the waste package is strongly influenced by the presence of water vapor and liquid water in the drift.

Once the waste package has been breached, the stainless-steel pour canister (for defense high-level waste forms) and Zircaloy cladding (for commercial and defense spent nuclear fuel) are exposed to the environment outside of the waste package, with one notable exception. Although the gaseous conditions (humidity, oxygen, and carbon dioxide content) will quickly equilibrate across the small holes in the waste package, the liquid phase conditions may be significantly different for very long time periods depending on the degradation characteristics at the surface of the waste package (size of openings, number of openings, and corrosion products filling the openings), the location and magnitude of any drips in the drift and the presence of any drip shields to intercept and shed the dripping water. Depending upon the expected environment inside the waste package following the breaching of the waste package containment barrier, the physical/chemical degradation of the cladding and pour canister will commence. The degree of degradation of these secondary containment barriers will affect the amount of radioactive material that is exposed to the environment in the waste package.

Once the waste form (whether glass or spent fuel) is exposed to the environment it can be altered. The degree and rate of alteration of the waste form are dependent on the local environment present at the waste-form surface, most notably the hydrologic and chemical conditions and the temperature. The hydrologic conditions on the surface of the waste form may range from humid air to adsorbed monolayers of water to a thin water film to some local film flow of water. The percent of the waste-form surface exposed and in contact with water will determine the rate at which radionuclides are released from the solid phase to the mobile liquid phase. It is the small subset of the total water flow that actually comes into contact with the waste that will ultimately determine the rate at which radionuclides are released.

Once radionuclides are released to a more mobile phase, they are available for transport. The transport mechanism depends on the distribution of water on the waste-form surface and between the waste-form surface and the outer edge of the degraded waste package. Given the low probability that there is a continuous advective flow of water along the waste-form surface (due to the low probability of any dripping water actually entering the waste package), the primary transport path will be by diffusion through a partially connected water film surface. The diffusion rate will be dependent on the water content within the waste package (i.e., the degree of interconnectedness of the water film), the water content within the corrosion products on the waste-package surface, the degree to which the waste-package surface has been corroded (i.e., the distribution of openings on the waste-package surface), and the concentration of the dissolved radionuclides at the waste-form/water contact (the concentration being a function of the rate of waste form alteration combined with the solubility of the radionuclide in the aqueous phase, which is in turn dependent on the local geochemical environment in the liquid on the waste-form surface). If pendular water can drip into the waste package, then it is possible to imagine an advective transport of radionuclides to the edge of the waste package. In general, because the mass release rate of radionuclides released by diffusive transport mechanisms is much lower than advective transport mechanisms, the degree to which water flows into the waste package is very important.

Once any dissolved radionuclides are transported to the edge of the waste package, the hydrologic and geochemical conditions within the degraded materials in the drift control the release of radionuclides to the host rock. If the probability of seepage into the drifts is low (due to the capillary forces in the rock tending to preferentially keep the liquid water in the rock rather than have it seep into the drift), then the primary transport mechanism in the drifts will be by diffusion. The diffusion rate will be dependent on the water content of the materials in the drift—the higher the water content, the more interconnected will be the water film surface, and therefore the transport path, and the greater the effective diffusion rate (Conca and Wright, 1992). For those cases where some water actually drips into the drift (although it may not have seeped into the waste package itself), the water will be able to advectively transport any dissolved radionuclides at a much greater rate than if only diffusive processes exist. For the design alternative of using a drip shield in the drifts, the objective is to minimize the chances that any water drips can advectively transport radionuclides. Also, in order to minimize the diffusion rate, backfill materials with a low residual water saturation (such as quartz sand) could be emplaced beneath the packages. Capillary equilibrium between the tuff host rock and the sand would constrain the sand to be at residual saturation.

It is worthwhile to point out that a drip-shield combined with a sand backfill diffusive barrier (not in the base case design) in the unsaturated zone at Yucca Mountain is analogous to the use of a bentonite backfill design in potential repositories being investigated in saturated crystalline rocks. The goal in both cases is to assure long transit times and slow release rates by diffusion along tortuous paths. In the case of unsaturated media, especially unsaturated materials in the drift, these tortuous paths involve discontinuous water film pathways. In the case of bentonite backfills these tortuous paths are the result of a discontinuous pore structure and restricted flow paths. The use of drip-shields or backfill in an unsaturated host rock for a repository has the potential additional benefit of keeping liquid water away from the waste package for the design life of the material.

4.2.4 Water Movement beneath the Repository Horizon

Once the radionuclides are transported through the engineered barriers and released to the rock, they may be advectively transported through the geosphere. Those radionuclides that may have been transported through the engineered barriers in gaseous form may continue to be transported in the gas phase in the unsaturated zone, but are more likely to be dissolved in the water that surrounds the drift and to subsequently be transported in the aqueous phase. The rate of transport through the unsaturated zone is dependent on the velocity of the ground water (which is in turn dependent on the degree of fracture flux in the different stratigraphic units, the liquid saturation within the fractures and matrix and the effective porosity of the fractures and matrix), the degree to which radionuclides may diffuse from the fractures into the matrix along likely travel paths, and the degree of adsorption of the different radionuclides on the mineral grains of the rock matrix or the fracture coatings. The velocity distribution may be locally quite heterogeneous in the unsaturated zone, which may be approximated using an effective dispersion within and between different lithologic units. This dispersion will tend to spread the arrival of any dissolved constituents, including any dissolved radionuclides, as they are transported through the unsaturated zone to the water table.

Although the transport through the unsaturated zone may be affected by the thermal perturbation caused by the emplaced waste, in general, past TSPAs have indicated that by the time any wastes are released to the geosphere, the hydrologic conditions have returned to almost the ambient flow system, so these thermal effects can probably be ignored. In summary, the amount of water moving in the host rock is significantly greater than the small amount of water in the drift and in contact with the radioactive waste. This water, and any dissolved radionuclides, must migrate about 300 m vertically in the unsaturated zone before it comes into contact with the flowing water in the saturated zone beneath the water table.

4.2.5 Water Movement in the Saturated Zone

Once the water in the unsaturated zone, and any dissolved radionuclides, reaches the water table, the radionuclides may be transported essentially horizontally in the saturated zone. The lateral flow in the saturated zone in the vicinity of Yucca Mountain is primarily in a southerly direction to the ultimate discharge of these waters to pumping wells in the Amargosa Valley or to natural discharge at Franklin Lake Playa or Death Valley. The lateral flow of water will first be through the fractured porous tuffaceous rock units immediately below the repository footprint (the saturated equivalents of the same lithologic units which exist above the water table). After about 10 km of lateral flow in the tuffaceous rocks, the ground-water flow will be in the thick alluvium of the Amargosa Valley. The lateral flow of ground water beneath Yucca Mountain is controlled not only by the recharge of water at Yucca Mountain itself but also by the significantly greater recharge of water from further north. (The recharge to the north is greater because the elevations are higher, so there is more precipitation and more infiltration.) That is, the water that started at the surface of Yucca Mountain and migrated through the unsaturated zone to the water table is now mixed with a significantly greater volume of water that started its journey further to the north. This mixing reduces the concentration of any dissolved constituents, potentially including radionuclides.

As in the case of flow and transport in the unsaturated zone, the velocity distribution beneath the water table will be heterogeneous in both magnitude and direction, which will tend to spread (e.g., disperse) any dissolved radionuclides both parallel and perpendicular to the average flow direction.

In addition to this spreading, some of the dissolved radionuclides will continue to be adsorbed on the mineral grains in contact with the flowing water. These processes will tend to further reduce the dissolved concentration of the radionuclides in the water which reaches any receptor well down gradient from the site.

Once the water traverses the distance between where it first enters the saturated zone to likely locations of human populations, the water may be extracted for various uses. These uses may include irrigation, bathing, drinking, and other potential biosphere pathways that describe how the water moves once extracted from the ground. Given that the water may contain some amount of dissolved radionuclides, these radionuclides may find their way into the food chain and ultimately be ingested by humans. Given that a portion of the radionuclides may be ingested, they may cause a radiation exposure (i.e., dose) to the population that consumes the food products and water. These doses may be compared to the background doses that these same individuals receive from all natural sources of radiation, including cosmic sources, radon gas emitted from surface soils, wind blown dust particles and ground water.

4.2.6 Summary of Processes that Affect Water Movement (and Radionuclide Transport)

We have now completed the journey of water as it migrates from rainwater which falls on Yucca Mountain through its ultimate discharge at pumping wells in the Amargosa Valley. To recap the processes that water has experienced along the way, we present the following list. These processes need to be evaluated and quantified in the prediction of the behavior of the natural and engineered components that affect total system performance.

Key Processes Defining the Behavior of the Undisturbed Yucca Mountain Repository System

- Precipitation
- Net Infiltration
- Unsaturated Zone Flow
- Mountain-Scale Thermal Hydrology
- Drift-Scale Seepage
- Drift-Scale Thermal Hydrology
- Drift-Scale Thermal Chemistry
- Waste Package Degradation
- Cladding Degradation
- Waste Form Degradation
- Radionuclide Mobilization
- Radionuclide Transport in the Engineered Barriers
- Radionuclide Transport in the Unsaturated Zone
- Radionuclide Transport in the Saturated Zone
- Radionuclide Transport in the Biosphere

4.3 *WHAT* IS BEING ANALYZED IN TSPA-VA

Having discussed in the previous sections *how* the repository is intended to perform and *what* physical-chemical processes affect the performance of the various engineered and natural barriers, we are now in a position to present *what* key attributes of the total system need to be addressed in TSPA-VA. Not surprisingly, the two aspects of *how* the repository is intended to perform and *what* needs to be analyzed are closely linked. If an aspect is important to the intended performance of the system then it needs to be included in the analysis. The details of how we intend to perform the analyses are described in Chapters 5, 6, and 7.

The key processes affecting potential repository performance at Yucca Mountain have been listed at the end of the previous section. A schematic depiction of these key processes is illustrated in Figure 4.3-1. This influence or bubble diagram illustrates the general logic and information flow in the TSPA analyses (illustrated in greater detail in Figures 7.1.2, 7.2.1, and 7.2.4). (The details of each of these "bubbles" or processes are described in the various sections of Chapter 6.) It is important to note that these illustrations of TSPA-VA information flow concentrate on the "expected" behavior of the system and the anticipated response of the natural system to the emplacement of radioactive materials at Yucca Mountain. In addition to the "expected" behavior, a number of "unexpected" (i.e., low probability) features, events, and processes (FEPs) need to be evaluated as well. Such potentially disruptive FEPs include volcanism, tectonism, human intrusion, and criticality. These will be evaluated with a series of discrete consequence analyses, as discussed in more detail in Sections 5.2.6 and 6.10.[2]

In light of the discussion in previous sections, Table 4.3-1 enumerates all the relevant components that need to be considered in the TSPA analysis and the key information which is passed from component to component. Each component essentially corresponds to a process which needs to be described quantitatively in the form of a model. These models (commonly referred to as process models) are described in greater detail in Chapter 6, with appropriate reference to the technical bases of these models (derived from laboratory or *in-situ* observations and tests), the uncertainty in these models that needs to be evaluated within the context of its significance to overall system performance, and the abstractions or simplifications to these process models as required for multi-realization probabilistic safety analyses.

[2] Although it is sometimes difficult to draw a clear demarcation between a FEP that is "expected" versus one that is believed to be of such a low likelihood of occurring that we may consider it "unexpected", we have chosen to term FEPs with an annual probability of 10^{-6} or less to be "unlikely". This corresponds to a probability of 0.01 over a 10,000 year time period. Given this definition, climate changes are expected to occur, as are seismic events of varying magnitudes, while volcanism, major tectonic events, and criticality are "unexpected". [FEPs with an annual probability of less than 10^{-8} are not considered to be sufficiently credible to warrant inclusion in the TSPA-VA analysis. Therefore, the "unexpected" volcanism, tectonism, and other disruptive events must have a probability in the range of 10^{-6} to 10^{-8} in order to be included.]

In the following section we outline the relationship of the key process models that must be analyzed in TSPA with the hypotheses identified in DOE's Waste Containment and Isolation Strategy (DOE,1996) as well as NRC's Key Technical Issues.

4.4 RELATIONSHIP OF TSPA COMPONENTS WITH DOE'S WASTE CONTAINMENT AND ISOLATION STRATEGY AND NRC'S KEY TECHNICAL ISSUES

The waste containment and isolation strategy (WCIS) (DOE, 1996) was developed to assist the Yucca Mountain Project in prioritizing testing and analysis activities to focus on the most important remaining issues regarding postclosure safety. The WCIS is designed to help resolve uncertainty in the processes and parameters of greatest significance to long-term performance and focuses on those attributes of the repository that are thought to have the highest probability of being reasonably bounded prior to the Viability Assessment. Although the WCIS is evolving, the discussion here is based on the documented version published by DOE in 1996. The following presentation will be revised if the WCIS is revised.

The WCIS (DOE, 1996) has identified five major system "attributes" that are the most important for performance assessment of the natural and engineered barriers:

(1) Rate of water seepage into the repository
(2) Waste-package lifetime (containment)
(3) Rate of release (mobilization) of radionuclides from breached waste packages
(4) Radionuclide transport through engineered and natural barriers
(5) Dilution in the saturated zone below the repository

A more detailed description of the WCIS attributes is as follows. The seepage rate attribute (i.e., slow groundwater movement) provides multiple functions, including limited water seepage from the host rock into the emplacement drifts (i.e., limited drips on the waste packages, which reduces the dissolution rate of the waste form and may reduce corrosion) and slow groundwater velocity throughout the unsaturated zone, which retards the arrival of radionuclides at the water table. The containment attribute provides for relatively long-term containment of the wastes (thousands of years) so long as the corrosion/degradation rate of the waste packages is sufficiently small. The waste-form mobilization attribute provides additional containment of the radionuclides due to the presence of the spent fuel cladding, as well as low dissolution rates and low solubility of some of the dissolved radionuclides, such as neptunium-237. The transport attribute has an effect in both the near-field (i.e., the EBS) and the far-field (unsaturated zone beneath the repository horizon). In the EBS it takes advantage of the limited amount of seepage into the drifts and the waste package, as well as potentially providing for adsorption of dissolved radionuclides. In the unsaturated zone (UZ), transport provides for the delay in migration of radionuclides to the saturated zone as a result of advective transport, retardation, and matrix diffusion, as well as dispersion, which reduces the peak concentration. The dilution attribute results in reduced concentrations (doses) as a result of large-scale mixing and dispersion in the saturated zone. Of the five system attributes discussed above, the seepage-rate attribute affects three of the others— containment, mobilization, and transport—so its effect must be represented in several of the process models.

In order to better evaluate the effect of the five system attributes on repository and subsystem (component) performance, a series of twelve working hypotheses have been formulated as a way to guide the testing and modeling of the physical-chemical processes associated with the various attributes. Specific hypotheses are associated with specific repository attributes as follows (DOE, 1996):

• *Rate of water seepage into the repository*

1. Percolation flux at repository depth is significantly less than net infiltration.
2. Fracture flow occurs within a limited volume of the repository host rock at any given time.
3. Seepage into the emplacement drifts will be limited to a small fraction of the incident percolation flux.
4. Bounds can be placed on thermally-induced changes in seepage rates.
5. Impacts of climate change on seepage rates can be bounded.

• *Waste-package lifetime (containment)*

6. Heat produced by emplaced waste will reduce relative humidity in the vicinity of waste packages.
7. Corrosion rates are very low at low relative humidity, and corrosion of the inner barrier is slow.
8. Double-walled waste packages will significantly increase containment times due to galvanic protection of the inner barrier by the outer barrier.

• *Rate of release (mobilization) of radionuclides from breached waste packages*

9. Radionuclide release from waste forms due to surface area exposed, dissolution, colloid formation, and microbial activity will be low.

• *Radionuclide transport through engineered and natural barriers*

10. Transport properties of both engineered and natural barriers will significantly reduce radionuclide concentrations due to depletion, diffusion and dispersion.

• *Dilution in the saturated zone below the repository*

11. Flow in the saturated zone is much greater than the flow contacting the waste.
12. Water percolating down through the repository horizon to the water table mixes with the flow in the aquifer.

In addition to the above twelve hypotheses, which are applicable for the nominal or "expected" performance, three additional hypotheses have been formulated for disturbed performance (disruptive events):

• *Disruptive events*

13. The amount of movement on faults through the repository horizon will be too small to bring waste to the surface, and too small and infrequent to significantly impact containment during the next few thousand years.
14. The severity of ground motion expected in the repository horizon for tens of thousands of years will only slightly increase the amount of rockfall and drift collapse.
15. Volcanic events within the controlled area will be rare and the radiological consequences of volcanism will be acceptable.

Table 4.4-1 shows the direct correspondence between process-level models being used for performance assessment and the fifteen WCIS hypotheses to be tested with these models.

The waste containment and isolation strategy acknowledges the uncertainty in our understanding of the natural and engineered components of the repository system and strives to place more reliance on those barriers that have been (or will be by the completion of TSPA-VA) best characterized. On the other hand, the Nuclear Regulatory Commission (NRC), tends to concentrate on those issues that are least well known, rather than the ones that are best characterized. This focus on uncertainty is conditioned, however, by the NRC staff's acknowledgement that importance to safety was and is being considered in the approach being adopted for KTI resolution. These NRC concerns/uncertainties are formally designated as Key Technical Issues (KTIs). Following is a list of the ten NRC KTIs:

1. Support revision of EPA standard/NRC rulemaking
2. Total system performance assessment and technical integration
3. Igneous activity
4. Unsaturated and saturated flow under isothermal conditions.
5. Thermal effects on flow
6. Container life and source term
7. Structural deformation and seismicity
8. Evolution of near-field environment
9. Radionuclide transport.
10. Repository design and thermal-mechanical effects

TSPA-VA will seek to address KTIs (2) through (10) through both process-level models, abstractions of process models, and total system performance models. Where possible, the KTIs will be directly included in process models. Otherwise, their effects will be incorporated in TSPA models statistically. Table 4.4-1 lists the correspondence between the NRC KTIs, the WCIS hypotheses, and the process models (and abstractions thereof) that seek to address these issues.

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Table 4.3-1. Information Flow Between Key Process Models in TSPA-VA

Process Model	Key Results
Climate model	Precipitation (t)
Infiltration model	Net infiltration (t)
Site-scale UZ hydrology model	Percolation flux at repository (t)
Repository-scale thermo-hydrology model	Average saturation at repository (t); Average percolation flux at repository (t)
Drift-scale thermo-hydrology model	Temperature (t); Invert liquid saturation (t); Relative Humidity (t)
Seepage model	Average seepage flux (t); Percent of repository area with seeps (t); Percent of total flux that seeps (t)
Drift-scale thermo-chemical model	Average pH, pCO_2, CO_3 in drift (t) Average pH, pCO_2, CO_3, Cl on waste package (t) Average pH, pCO_2, CO_3, F, Si, PO_4, SO_4 on waste form(t)
Drift-scale thermo-mechanical model	Change in hydrologic properties (t); Distribution of rock falls (t)
Drift-scale T-H-M-C model	Temperature (t); Relative Humidity (t); Average seepage flux (t)
Waste package degradation model	Number of pits through corrosion allowance material (t); Number of pits through corrosion resistant material(t), Degradation rate of corrosion allowance material(t); Degradation rate of corrosion resistant material (t); Percent of waste package surface with pits (t)
Cladding degradation model	Percent of cladding with pinholes (t); Percent of cladding unzipped (t)
Inventory model	Radionuclide activity in place (t)
Waste form degradation model	Surface area exposed (t); Surface area wetted (t); Radionuclide activity release rate from altered waste form (t)
Radionuclide mobilization model	Radionuclide activity release rate to mobile phase (t); Percent of radionuclide activity in mobile phase (t)

Table 4.3-1. Information Flow Between Key Process Models in TSPA-VA (Continued)

Process Model	Key Results
Drift-scale transport model	Radionuclide activity release rate to UZ (t); Percent of radionuclide activity released to UZ (t)
Site-scale UZ transport model	Radionuclide activity release rate to SZ (t); Percent of radionuclide activity released to SZ (t)
Site-scale SZ flow & transport model	Radionuclide activity release rate to AE(t); Percent of radionuclide activity released to AE (t); Average radionuclide concentration at AE (t); Peak radionuclide concentration at AE (t)
Biosphere transport model	Dose to average member of critical population (t); Percent of radionuclide activity ingested/inhaled (t)
Tectonic effects model	Probability Change in hydrologic properties
Volcanic effects model	Probability Change in hydrologic, thermal and waste package degradation
Criticality effects model	Probability Change in inventory and thermal properties

(t) indicates information that is temporally dependent

Table 4.4-1. Correspondence of Key TSPA-VA Process Models to Waste Containment and Isolation Strategy (WCIS) Hypotheses[1] and NRC Key Technical Issues (KTIs)[1]

Process Model	WCIS Hypothesis	NRC KTI
Climate change model	5	4,5,9
Infiltration model	1, 2, 3	4
Site-scale UZ hydrology model	1,2,3	4
Repository-scale thermo-hydrology model	4	5
Drift-scale thermo-hydrology model	4,6	5,10
Seepage model	4	4
Drift-scale thermo-chemical model	9,10	5,8
Drift-scale thermo-mechanical model	2	10
Drift-scale coupled T-H-C-M model	9,10	5,6,8,10
Waste package degradation model	7,8	6
Cladding degradation model	9	6
Waste form degradation model	9	6
Radionuclide mobilization model	9	6,8
Drift-scale transport model	10	9
Site scale UZ transport model	10	9
Site-scale SZ flow model	11,12	4
Site-scale SZ transport model	12	9
Biosphere transport model	n/a	9
Tectonic effects model	13,14	7
Volcanic effects model	15	3
Criticality effects model	n/a	n/a

[1] See text for descriptions of WCIS hypotheses and KTIs.

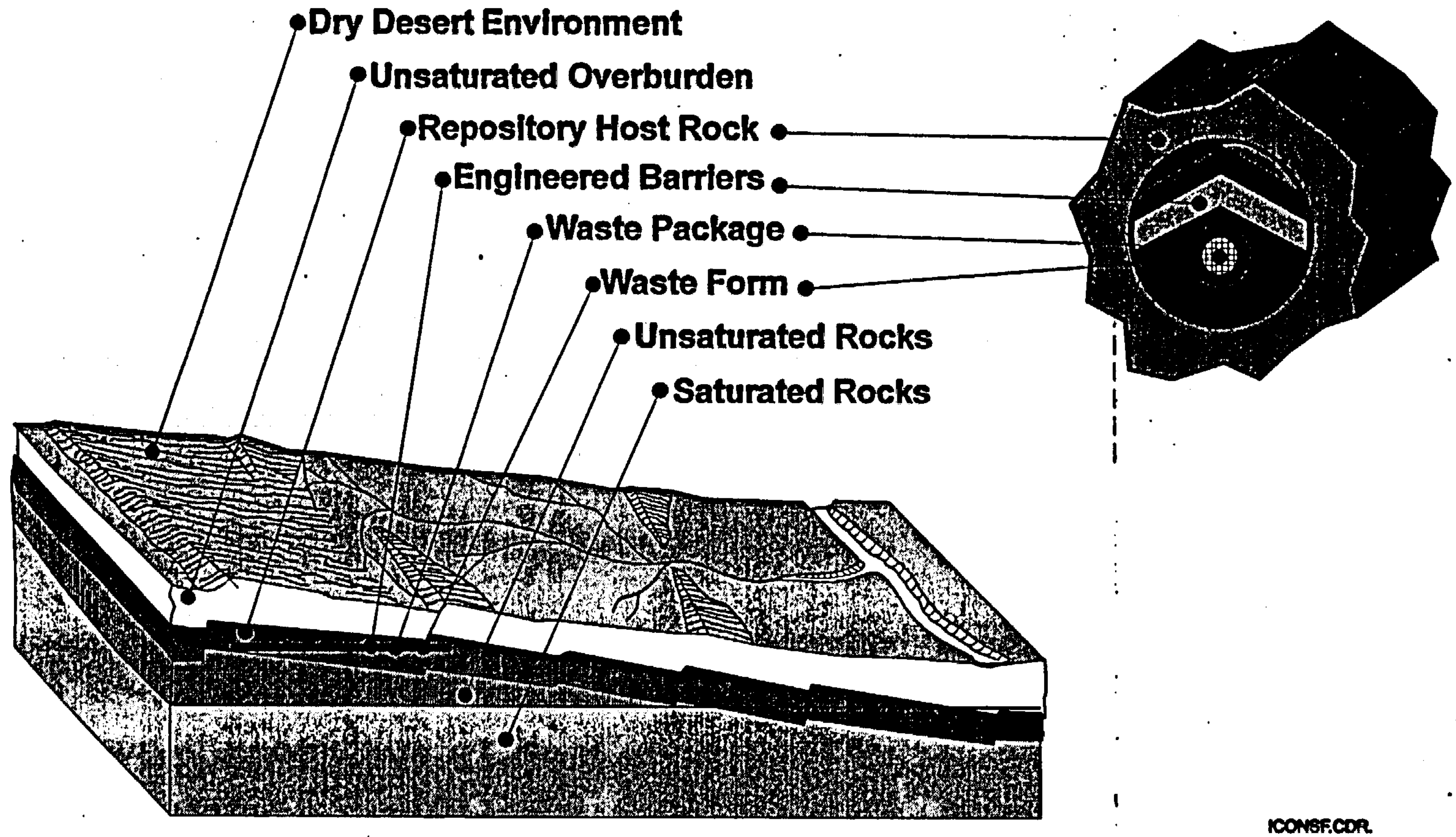

Figure 4.1-1. Schematic of Components Affecting Total System Performance

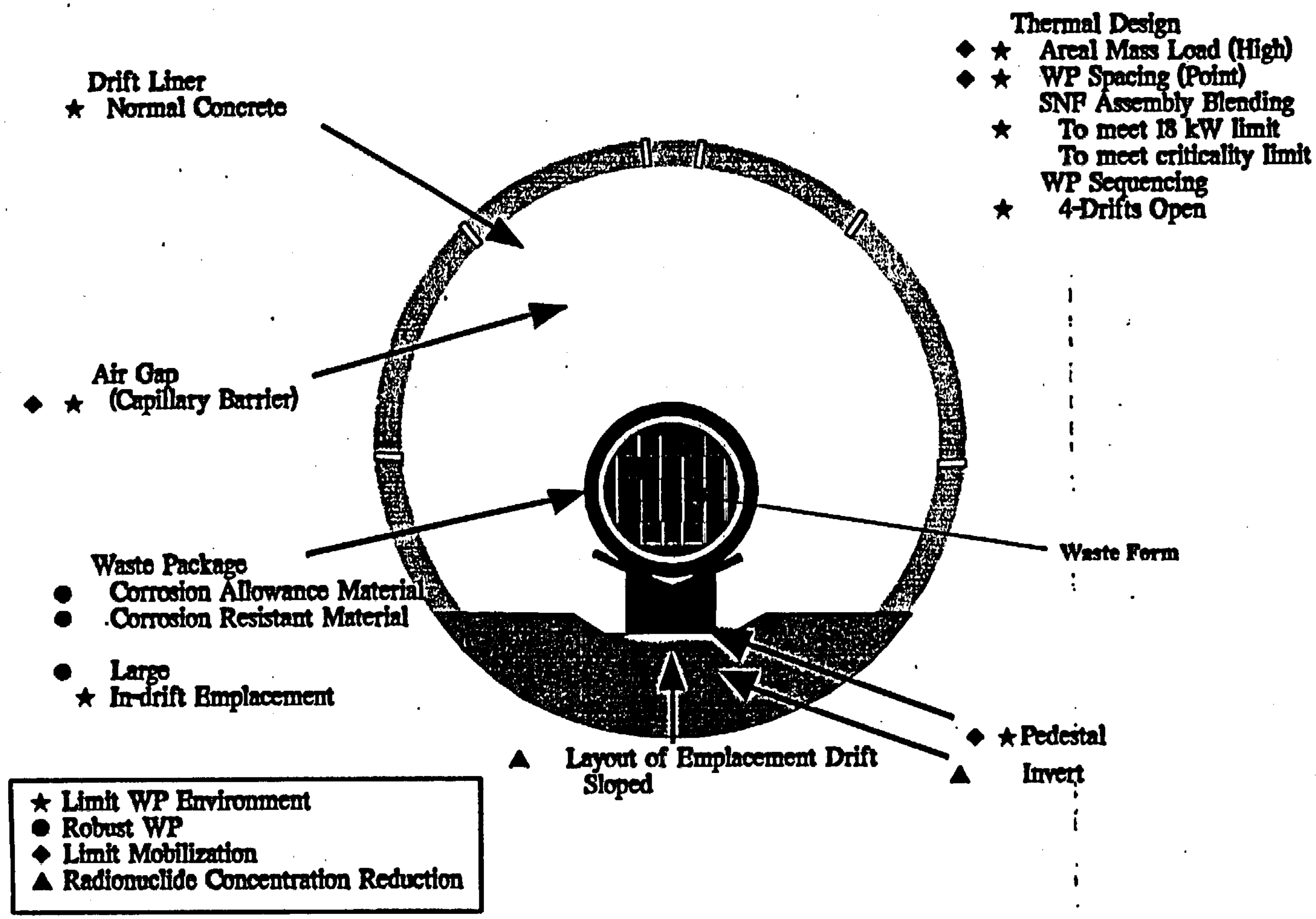

Figure 4.1-2. Base Case Design for TSPA-VA (after M&O, 1997b)

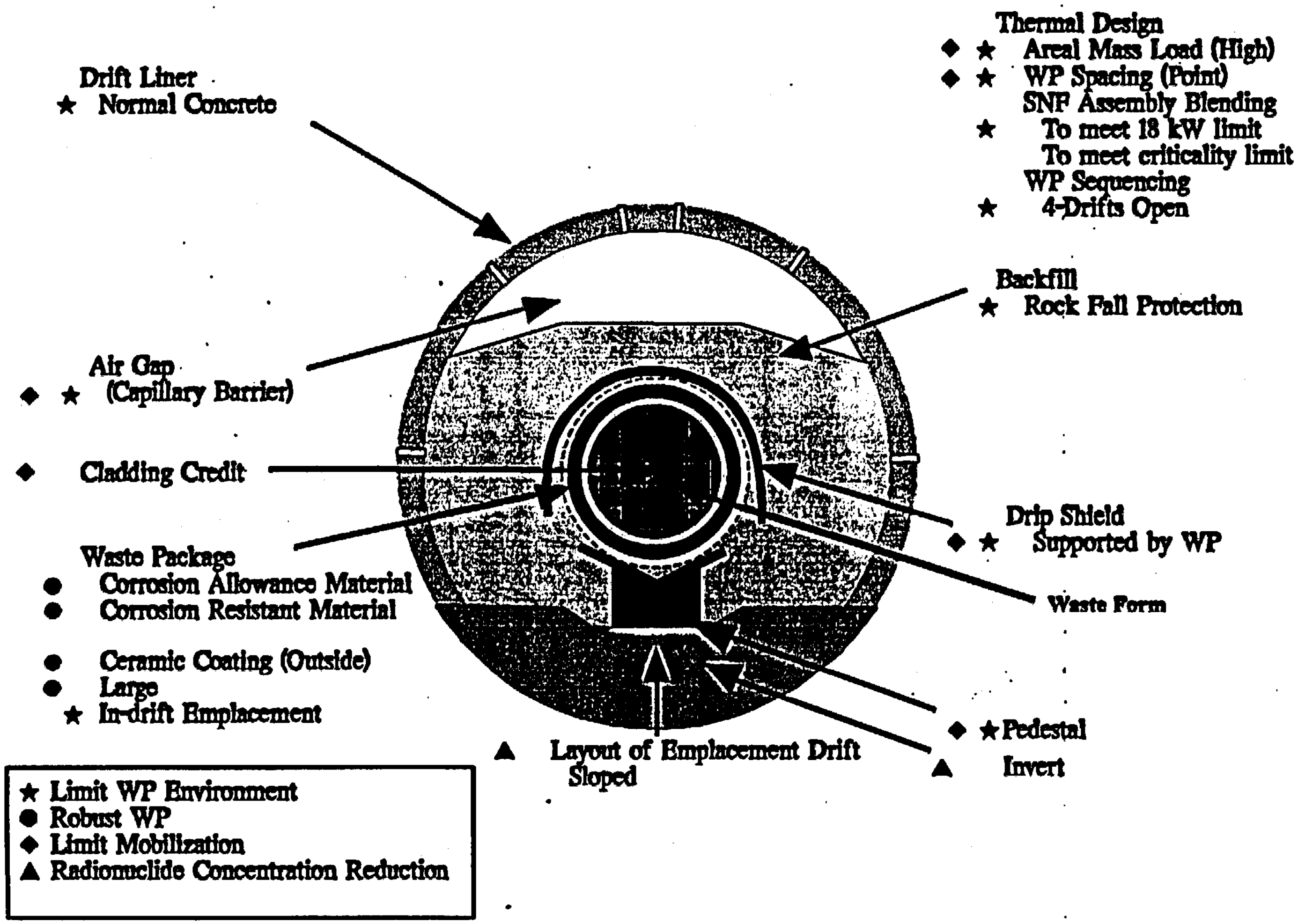

Figure 4.1-3. Design Options presented on Base Case Design (after M&O, 1997b)

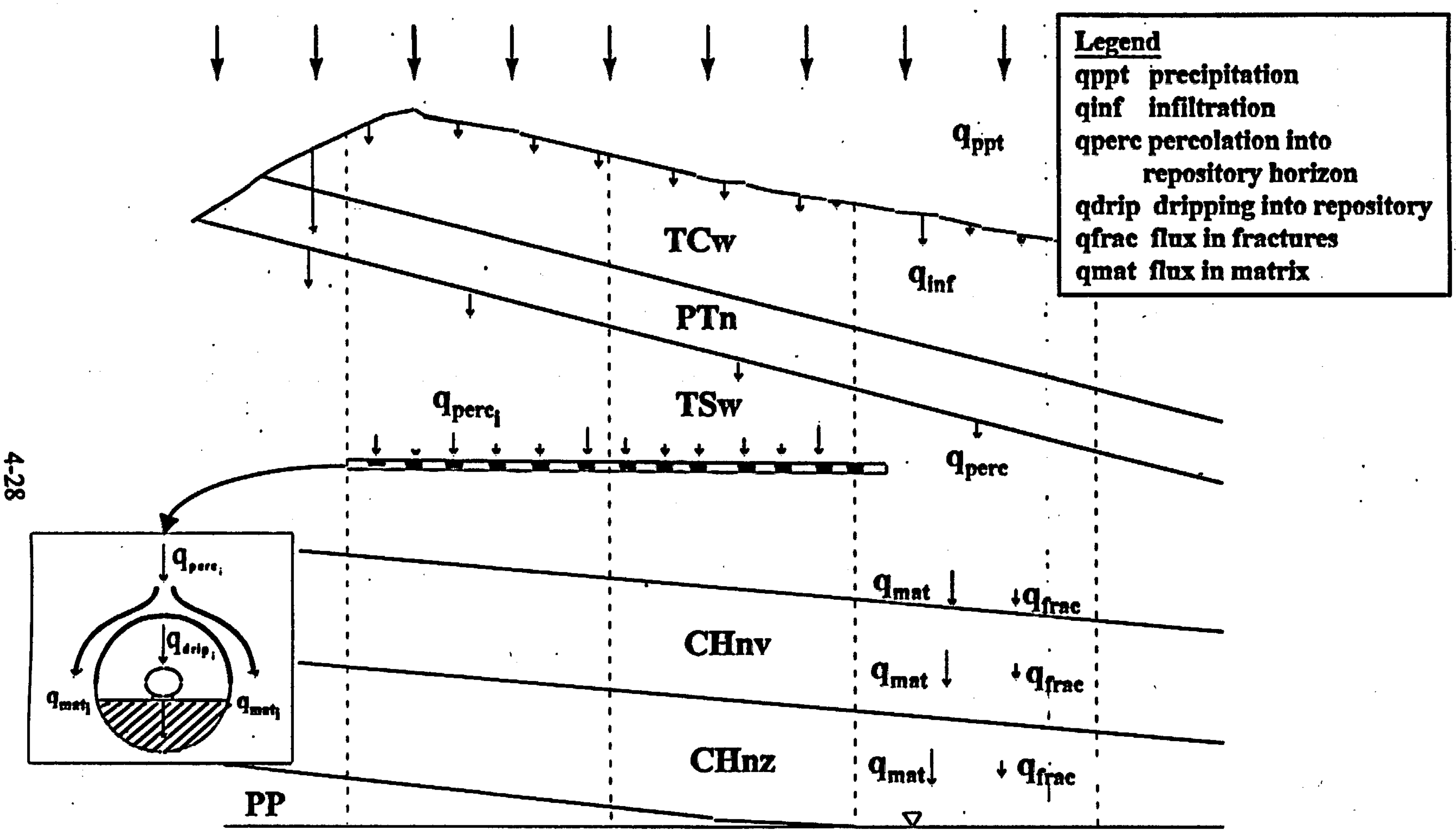

Figure 4.2-1. Conceptualization of Flow Through the Natural and Engineered Systems at Yucca Mountain

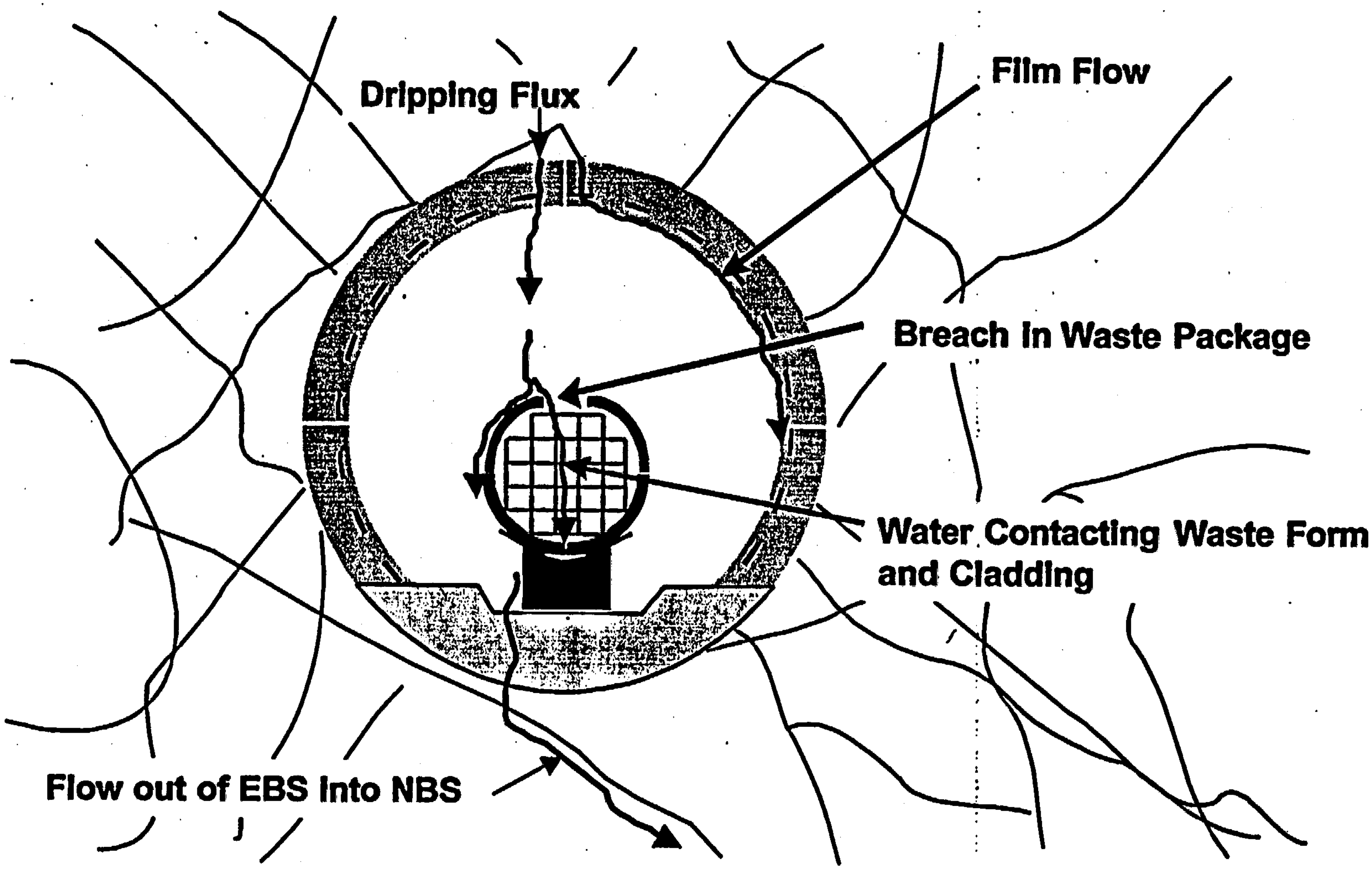

Figure 4.2-2. Schematic of Potential Water Flow in the EBS

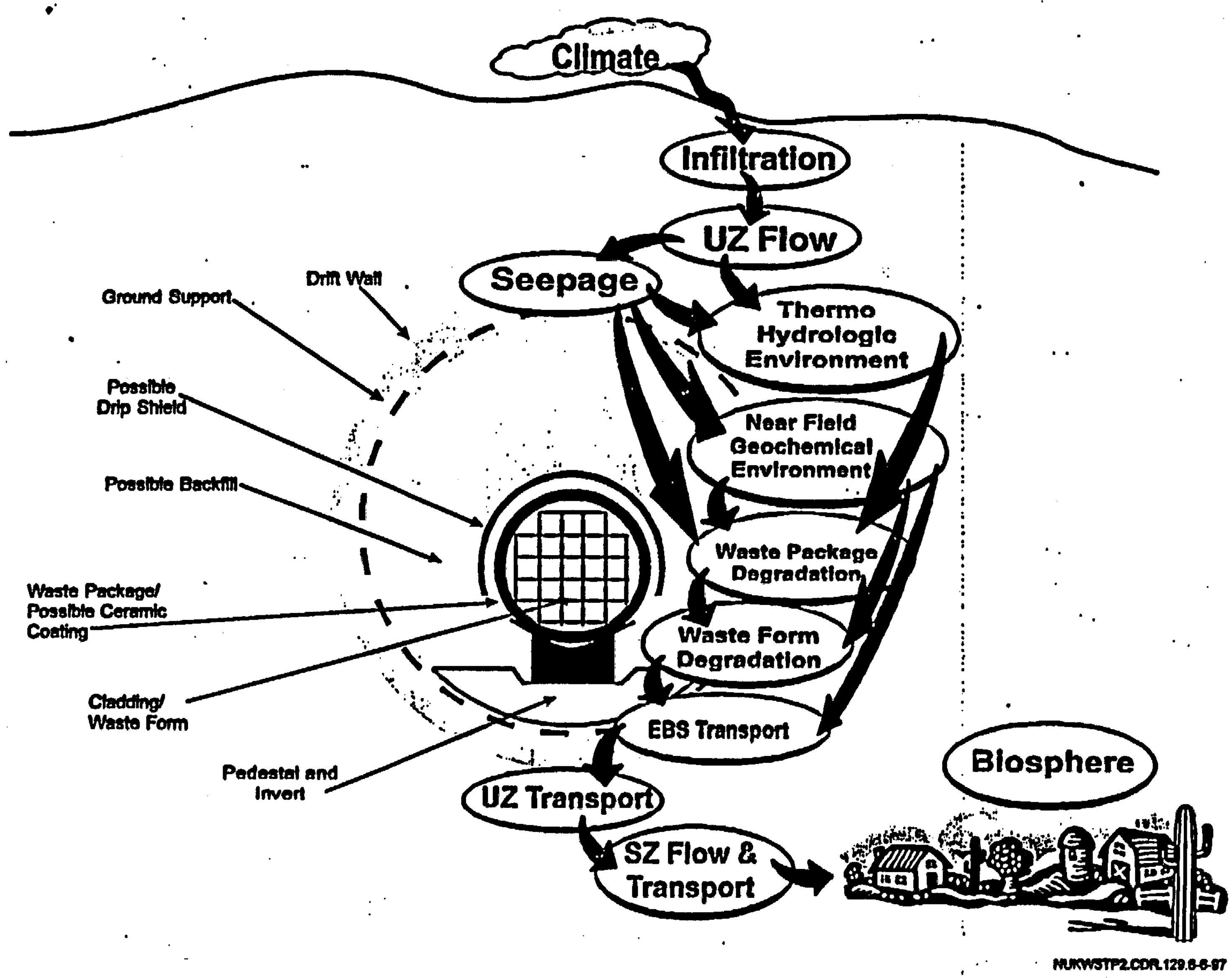

Figure 4.3-1. Models for Total System Performance Assessment

5.0 TSPA-VA GENERAL APPROACH AND METHOD

Robert W. Andrews, S. David Sevougian

5.1 INTRODUCTION

Having described in the previous chapter *what* components must be included in an assessment of total system performance, it is now appropriate to discuss *how* the TSPA for the Viability Assessment is intended to be performed. Although not all the details are defined at this time, sufficient information is available to afford the reader the opportunity to understand first the general approach and methodology described in this chapter, followed by more detailed discussions of the abstraction of the individual process models presented in Chapter 6 and the inputs of these abstracted models in the TSPA software described in Chapter 7.

Prior to discussing the general approach, it is worthwhile to recall the language of the 1997 Energy and Water Appropriations Act, which defines the overall scope and objectives of TSPA-VA:

> "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"

From this objective, the major inputs to the performance assessment can be seen to be the design concept, the scientific data and analysis, and the overall system performance standards. Each of these inputs is described in general terms in the following paragraphs.

The design concept used as input to the TSPA-VA consists of the subsurface repository layout, the engineered barrier segments and the waste package. The definition of the repository layout includes the lithologic unit(s) that will comprise the host rock for the repository, the depth and areal extent of the facility, the drift size and spacing, the mechanical support system to be employed, the thermal load, and the ventilation system used during the operational phase of the facility. The definition of the engineered barrier segments includes the invert and pedestal systems to be used to support the waste package, the potential use of any packing or backfill materials within the drift, and the potential use of any drip shield placed over or around the waste package. The definition of the waste package includes the size and thermal characteristics (including the number of spent-fuel assemblies or DHLW glass logs to be emplaced in each waste package), the materials to be used including the potential use of any coatings placed around the waste package, and the techniques to be employed in the fabrication and inspection of the waste packages. All of these inputs are being provided by the design organization through a controlled process (see Section 7.1.3).

The scientific data and analysis used as input to the TSPA-VA consists of models (and their associated parameters) of the key processes described in Chapter 4 and the technical bases for these models. The technical bases of these models is dependent on laboratory and *in-situ* observations and tests. The scientific process models may be generally subdivided into those related to geosphere processes and those that relate to engineered barrier system processes. The key geosphere processes include climate change, unsaturated zone hydrology, thermal hydrology, thermal chemistry, unsaturated zone radionuclide transport, saturated zone hydrology and radionuclide transport, biosphere transport, volcanism, and tectonism. The key engineered barrier system processes include in-drift thermal hydrology and thermal chemistry, degradation of any potential drip shield or ceramic coating (not in base case), degradation of the waste package, degradation of the cladding, alteration and dissolution of the waste form, degradation of the invert, mobilization of the radionuclides, and transport of the radionuclides in the drift. All of these inputs are being developed by the site and design organizations using a documented process.

At present (August 1998), there are no specified overall system performance standards to which the probable behavior of the Yucca Mountain repository system can be compared. In order to move forward to the Viability Assessment in the face of regulatory uncertainty, the YMP has prepared an internal system-level performance measure that is to be used until such time as the U.S. Environmental Protection Agency issues a Yucca Mountain specific standard as directed by the U.S. Congress. This interim performance measure and goal are reproduced below:

> **General**
> The interim system-level performance measure is a quantitative statement of necessary performance for the first 10,000 years after closure. It is followed by a system-level performance goal that recognizes there needs to be sufficient defense-in-depth in the repository's multiple barrier system to ensure that public safety is protected beyond 10,000 years. This is a serious system performance goal. It is qualitative because of increasing uncertainties beyond the first 10,000 years.
>
> **Performance Measure**
> The expected annual dose to an average individual in a critical group living 20 kilometers (km) from the repository shall not exceed 25 mrem from all pathways and all radionuclides during the first 10,000 years after closure.
>
> **Goal**
> Conduct analyses beyond 10,000 years to gain insight into longer-term system performance. For this period, the expected annual dose to an average individual in a critical group living 20 km from the repository should be below the 10,000 year performance measure. (Barnes, July 14, 1997)

(While the DOE believes that the appropriate point of compliance, based on current-day characteristics of the region, should be at 30 km downgradient from the repository, 20 km was selected to provide additional conservatism.) Based on the above interim post-closure performance measure and goal, and using the Viability Assessment design concept and all available scientific data and analysis, we are now in a position to discuss the approach to be followed in TSPA-VA to evaluate the probable behavior of the repository in the Yucca Mountain geologic setting.

5.2 GENERAL APPROACH

The overall approach to TSPA-VA may be broken into the following eight activities:

1. Develop, substantiate, test and document models of all relevant processes affecting post closure waste containment and isolation, using input from scientific and design investigations.

2. Identify relevant uncertainties in process models.

3. Identify all relevant scenarios to be analyzed in the total system performance assessment.

4. Conduct sensitivity analyses on each of the key process models to determine the effects of all of the relevant uncertainties.

5. Abstract[1] the relevant results from the process models (including the uncertainty) to provide input to the total system model.

6. Conduct total system analyses that will predict performance.

7. Document all assumptions, results, and conclusions including those relevant to the prioritization of future site and design activities required to develop a more robust analysis for the License Application.

8. Conduct a Peer Review of the TSPA assumptions, results, and conclusions.

In the following paragraphs, we discuss the objectives within each activity enumerated above. As will be discussed in Chapter 7, many of these activities run concurrently and iteratively with the aim being to always focus our attention on those aspects that most significantly affect the prediction of post-closure performance and the traceability and transparency of those predictions.

A schematic depiction of the general approach used to generate an integrated assessment of post-closure performance is illustrated in Figure 5.2-1.

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[1] The abstraction of process model results is the method of simplifying the essential components of the process model in a suitable form for use in an assessment of total system performance. The simplification should retain the basic intrinsic form of the process model without requiring the complexity incorporated in the process model. Such model abstraction is required in order to maximize the utilization of finite computational resources while allowing a sufficient range of sensitivity and uncertainty analyses.

5.2.1 Develop, Substantiate, Test and Document Models of Relevant Processes

Any prediction of performance is predicated on the quantitative description of the key processes that must be included in that analysis. In Chapter 4, we presented the key process models that comprise the repository system at Yucca Mountain. These process models are illustrated in one of the boxes in Figure 5.2-1. For each of these process models, laboratory and *in-situ* tests and observations have been used to substantiate the current understanding of the expected behavior of each of these components of the system. In cases where specific test results are either lacking or are ambiguous with regards to their interpretation, formal expert elicitation has been conducted to assist in identifying the most reasonable models or parameters plus some quantification of the uncertainty in these models or parameters. These expert elicitations were conducted in accordance with the U.S. Nuclear Regulatory Commission Branch Technical Position (NRC, 1996).

5.2.2 Identify Relevant Uncertainties in Process Models

Although the focus of the Viability Assessment is on the "probable behavior" of the repository, we must acknowledge that the key processes and corresponding process models and parameters have associated with them varying degrees of uncertainty. This uncertainty can exist in either the applicable conceptual models used to describe the process or in the discrete parameter values used in the model. Developing reasonable quantitative estimates of the uncertainty is sometimes difficult and can be subjective. Recognizing this subjectivity is important and illustrates the need to evaluate the significance of this uncertainty.

An important issue in the prediction of a natural system response to an imposed stimulus is appropriately segregating uncertainty in the prediction, which is derivable from uncertainty in the underlying knowledge, from the natural intrinsic variability of the model or parameter. A few examples may help illustrate the difference. Numerous saturated matrix permeability values and water content values have been determined from laboratory measurements of core samples of the different lithologic units in the unsaturated zone at Yucca Mountain (Flint, in preparation). These measurements indicate a range of values. Although there is some uncertainty in the measurements themselves, the principal cause for the range of values is considered to be the result of natural variability from sample to sample which is presumed to be correlated with the expected variability in this property from location to location in the rock mass. This variability needs to be appropriately incorporated in the TSPA analyses. Greater uncertainty arises when the matrix permeability and water content values, measured on the scale of a few centimeters, are used to calibrate a flow model with grid blocks on the order of tens to hundreds of meters (Bodvarsson et al., 1997). This uncertainty with respect to the geometric scaling is compounded by the fact that the primary model prediction, the liquid flux, can not be directly measured at the field scale in the unsaturated zone at Yucca Mountain. Thus, various indirect, inferential methods are used to predict the liquid flux—based on other models and measurements such as the observed temperature gradient in the unsaturated zone.

A different example relates to the solubility of radionuclide species. Again, several laboratory measurements of solubility have been generated for a few key radionuclides (including neptunium) over a range of different chemical and thermal conditions (Triay et al., 1996). The values obtained indicate a variability from sample to sample. In addition to this variability, there is significant uncertainty concerning whether the tests have achieved local chemical equilibrium and what are the solid phases controlling the solubility measurements. This uncertainty needs to be addressed in the TSPA analyses.

Additional uncertainty may occur in the conceptual model(s) underlying the process-level model. An example is the use of dual permeability or equivalent continuum representation of the flow through the unsaturated zone.

With the aim at generating reasonable estimates of the major uncertainties in each of the key process models, we have used different approaches. As a first step we have conducted workshops on each process model with attendance from a representative cross section of Yucca Mountain Project scientists and engineers. One of the aims of these workshops was to identify the key uncertainties associated with each process model. Summaries of the results of these workshops are contained in the various sections of Chapter 6. Secondly, we have used input from various external review organizations, notably (1) the NRC and their contractor, the Center for Nuclear Waste Regulatory Analyses (CNWRA) [as documented in their audit review of TSPA-1995 (Baca and Brient, 1996), and the status of their analyses associated with the KTIs, as documented in the NRC's Annual Progress Report (Sagar, 1997)]; (2) the Nuclear Waste Technical Review Board [as documented in their Report to the U.S. Congress and The Secretary of Energy (NWTRB, 1997)]; and (3) most recently, the First Interim Report of the TSPA Peer Review Panel (Whipple et al., 1997). Finally, we have used formal expert elicitation of key aspects of the process models to assist us in quantifying uncertainty. To date expert elicitations of probabilistic volcanic hazards and unsaturated zone flow have been completed and documented in M&O (1996; 1997a), respectively. Ongoing elicitations include probabilistic seismic hazards, waste package degradation, and saturated zone flow and transport. The use of these elicitations is not to replace information on these process models generated from laboratory and field investigations, but to aid in the quantification of uncertainty given the available information.

5.2.3 Identify Relevant Scenarios to be Analyzed

The term "scenarios" has many different meanings. In the case of TSPA-VA, a scenario is a well-defined connected sequence of features, events, and processes (FEPs) that can be thought of as a possible future history of the repository system. Features are the geologic or hydrologic properties of the site or system, which are expected to be enduring. Processes are phenomena that have gradual, continuous interactions with the system. Events are occurrences that have a specific starting time, and usually a duration shorter than the time being simulated. FEPs are frequently organized into tree-like structures called event trees or FEP diagrams.

FEPs and scenarios can be divided into two types: "Undisturbed" or "disturbed". Undisturbed performance refers to the "nominal" behavior of the system as perturbed by "expected" events. Disturbed performance encompasses disruptive events such as human intrusion, igneous activity, seismic activity, and nuclear criticality, which may occur in addition to nominal evolution of the repository system. The effects of disruptive events can be of two types: direct release of radioactivity to the surface or alteration of the "nominal" behavior of the system.

Although event trees and FEP diagrams can be created for either disturbed or undisturbed scenarios, for the Yucca Mountain TSPA the focus of scenario analyses has been on addressing a range of "what-if" questions associated with low probability "unexpected" disruptive FEPs such as volcanism, tectonism, and criticality. The nominal evolution of the repository system, which may be described by the range of key model results indicated in Table 4.3-1, is best illustrated by a description of the "likely" evolution of the repository and wastes as a function of time after the repository is closed. As uncertainty exists in the likely evolution of the repository system, this uncertainty will be quantified and the effect on the predicted consequences evaluated in TSPA-VA.

In addition to identifying the range of alternative conceptual models that need to be evaluated in the context of TSPA-VA, an important goal of TSPA is to determine the potential benefits (in terms of reduced consequences to human health or the environment) of alternative repository and waste package design options. As noted in the Reference Design Description[2] (M&O, 1997b), a number of design options may be considered to either (1) delay the breaching of the waste package, (2) slow the release of radioactive materials from the waste package, or (3) retard the release of radioactive materials from the engineered barrier system. In addition to the performance-related implications, each of the design options has associated with it a potential cost and schedule impact. Managers and decision makers at all levels need to be apprised of the cost, schedule, and performance implications of different design options. The principal design options that are currently planned to be evaluated in TSPA-VA include: (1) the use of different waste package materials, (2) the use of ceramic or other impervious coatings on the waste package surface, (3) the use of a drip shield supported by the waste package, and (4) the use of backfill around the waste package. (This was previously discussed in Chapter 4.)

5.2.4 Conduct Sensitivity Analyses Using Each of the Key Process Models

In each of the key process models that ultimately feeds into the description of the total system, some uncertainty exists regarding the appropriate conceptual model or range of applicable parameter values that may potentially affect the predicted performance. Rather than include all of this uncertainty in the TSPA analyses themselves, sensitivity analyses have been designed to investigate

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[2] The Reference Design Description is expected to be updated with current information on a quarterly basis. The basis of the design concept to be evaluated as the "reference" design in TSPA-VA is to be completed by September 30, 1997. This will be documented in a revision to the Reference Design Document. Any changes in the design after September 30, 1997 and prior to the completion of the TSPA-VA are assumed to be minor in nature and more aimed at providing sufficient detail for cost estimates and, therefore, will not substantially impact the TSPA analyses.

the impact of these varying uncertainties on the results of the process models (see Sections 6.x.5). The philosophy we have taken is to first determine if, based on these sensitivity analyses, it can be demonstrated that the uncertainty has a minimum effect on some relevant surrogate of total system performance. If this is the case then there would be no need to propagate the effect of that uncertainty onto the total system performance. If, on the other hand, the parameter or conceptual model does have a significant effect on the surrogate of performance, then that parameter or model would need to be included in the TSPA analyses, either as a range of values to be sampled or as a discrete "sensitivity case" (see Sections 6.x.6 and 7.3).

The reason for conducting these process-based sensitivity analyses is primarily to focus our resources on the most significant issues. As noted above, the key issues have been identified using a number of different inputs from within the Yucca Mountain Project as well as external review organizations. Initial prioritization of these issues was accomplished during a series of workshops held with project scientists and performance assessment analysts and observed by members of these external organizations (cf. Chapter 2). Continued efforts to prioritize the issues, to be followed through the TSPA analyses themselves, are necessary to assure that the focus is and stays on those aspects of the system that most control the predicted dose.

5.2.5 Abstract the Relevant Results from the Key Process Models

Due to the uncertainty, variability, and complexity of the overall repository system and subsystems, it is generally necessary to make some simplifications to the process-level models for use in the TSPA analyses. One reason for this simplification is to allow a range of alternative hypotheses to be investigated in a reasonable amount of computational time using probabilistic methods analogous to those used in nuclear reactor safety analyses, commonly referred to as probabilistic risk analyses (PRAs). The abstract, probabilistic PRA approach is useful because of the inherent uncertainties in predicting the behavior of any geologic or man-made system many thousands of years into the future. In particular, there is always a degree of uncertainty and variability in both natural geologic and engineered systems, which when carried forward to predictions of future behavior, requires a probabilistic method. The hundreds of model realizations necessary to adequately characterize the probability distribution of future system behavior would require hundreds of computer simulations of the various process-level models. Because the simulations of the detailed process-level models are restricted by finite computer resources, some simplifications (here called "abstractions") are generally necessary.

For the purposes of TSPA, the word *abstraction* is used to connote the development of a simplified/idealized process model (with appropriately defined inputs) that reproduces/bounds the results of the underlying detailed process model. The inputs for the abstracted model can be either a subset of those required for the detailed process model or intermediate results from the detailed process model that have been analyzed to develop "response functions", which can then be used as inputs to the abstracted model.[3] In either case, it is necessary to demonstrate that predictions of both the detailed process model and the abstracted model are reasonably similar. A general discussion of various levels of abstraction is presented in Section 5.3. Detailed discussions of the abstraction activities for each of the key process models that will be included in the Yucca Mountain TSPA-VA are presented in Chapter 6, and a discussion of various abstractions as they impact the TSPA-VA model and code architecture is given in Section 7.2.

5.2.6 Conduct Total System Performance Analyses

Once the abstracted models have been developed, they must be appropriately linked in a computationally efficient manner to allow for the assessment of system behavior and performance. The software to be used in TSPA-VA will be an enhanced version of the software used in TSPA-1995, RIP (Repository Integration Program). A description of RIP can be found in Golder (1997). RIP essentially is an integrating software code, into which simplified analytical expressions or callable subroutines, describing the behavior of the different components, can be placed. RIP sequentially marches through time, keeping track of the changes in environments and the fate of the radioactive constituents within the engineered and natural barriers.

As the focus of TSPA-VA is on the "probable" behavior of the system as defined in the VA objectives, emphasis in the analyses will be on the "expected" models and parameters. However, a wide range of sensitivity and uncertainty analyses will be conducted to evaluate the significance of parameter and conceptual model uncertainty. Given this uncertainty it is difficult to precisely define the expected behavior. However, by conducting a full suite of sensitivity analyses and appropriately weighting the alternative models and parameters, the decision maker should be able to determine the degree of risk associated with different design decisions.

As mentioned in Section 4.3, for the purposes of TSPA-VA, a distinction between probable and unlikely FEPs will be drawn at an annual probability of 10^{-6} (corresponding to a probability of 0.01 over 10,000 years). These FEPs will not be included in the "nominal" or "expected" TSPA-VA analyses, but in order to address their consequences, a range of "what-if" analyses will also be conducted for these low probability FEPs; in particular the disruptive FEPs such as volcanism, tectonism, human intrusion, and criticality. Although we do not consider any of the above FEPs to be "expected" (i.e., with a probability greater than 0.01 over 10,000 years), their consequences, were they to occur, are often perceived to be significant, thus necessitating their inclusion in the analysis.[4]

Given a reasonable range of alternative models, it is possible to combine the results of individual sensitivity analyses into a global analysis using representative probabilities (e.g., weights) for each of the alternatives. Although we intend to conduct such combinations, we will also show the

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[3] These response functions (developed from the process model output) may themselves be the abstracted model.

[4] Climate change and seismic events of varying magnitude are considered to be "expected" and will be included in all TSPA-VA analyses.

individual results to give the reader a sense of which models and assumptions were most significant to the overall prediction. (See Section 7.3 for an elaboration of this idea.)

5.2.7 Document Assumptions, Results and Conclusions

One of the most crucial tasks in TSPA-VA is to produce a "transparent"[5] document detailing the assumptions, results, and conclusions. A critical aspect of this document is that the record of decisions and assumptions made in the analysis must be "traceable". As the TSPA models become more process-based (i.e., are more directly linked to process models), which is a natural progression as we include more representative models in the analysis, the degree of complexity increases. While this is a desirable trait in that it enhances the traceability of the analysis and the technical basis of the assumptions used in the analysis, it can lead to a reduced transparency. There is some recognition that a suite of TSPA analyses may be required at different levels of complexity to aid in the communication of the results and their implications. We are investigating various alternatives for the presentation of the results to assure that different audiences can find an appropriate level of detail in the explanations.

One method to illustrate the results of the system behavior is to examine in some detail the expected evolution of the individual components that feed into the overall system assessment. The key results of the models tabulated in Table 4.3-1 could be illustrated in a series of time varying responses. Of particular interest would be quantitative depictions of the release rate of radionuclides across different segments of the total system as a function of time, or the cumulative inventory (or percent of the initial inventory) contained within different components of the system as a function of time. Either of these latter plots would illustrate the effect of containment within the engineered barrier and the release rate across different barriers over time.

Given that parameter uncertainty will be a key aspect to be evaluated in TSPA-VA, various statistical measures of the uncertainty in the predicted results will be presented. As it may be difficult to grasp the effectiveness of complimentary cumulative distribution functions (CCDFs) as a means of quantifying the range of possible results, we will also employ probability density functions (PDFs). It may also be informative to present a few representative cases (such as various percentiles of the total distribution such as the 5th, 15th, 50th, 85th and 95th percentiles) and various intermediate level results (such as releases from different components of the system over time) to illustrate the range of possible outcomes (see Section 7.3.3).

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[5] Both the TSPA Peer Review Panel and the NWTRB have recently defined what they mean by "transparency". The Peer Review Panel, referencing a draft report of a subgroup of the Performance Assessment Advisory Group of the Paris-based Nuclear Energy Agency, noted that transparency "requires ensuring completeness and using a logical structure that facilitates in-depth review of the relevant issues". They continue to state that transparency "is achieved when a reader or reviewer has a clear picture of what was done in the analysis, what the outcome was, and why" (Whipple et al., 1997, pp 9-10). The NWTRB states that "transparency is the ease of understanding the process by which a study was carried out, which assumptions are driving the results, how they were arrived at, and the rigor of the analyses leading to the results" (NWTRB, 1997, p 21).

In order to illustrate those models and parameters that most significantly affect the predicted results, different post-processing techniques will be employed. These methods include graphical depictions such as scatter plots, where the impact of parameter x on the outcome y can be cross-plotted to illustrate any strong dependencies. Additional statistical analyses such as regression analyses can also aid in identifying the key parameters (see Section 7.4).

In addition to documenting the technical aspects of the TSPA analyses and the bases for the conceptual model and parameter assumptions made in the analyses, the TSPA-VA document will also describe how the information which flows through the series of TSPA models is controlled. This control, as described in Section 7.1, adds to the traceability of the analysis and enforces the integration of the scientific and engineering information used as a basis for the analyses.

A key utility of the documentation of TSPA-VA will be the identification of key information needs to make the TSPA-LA more complete and defensible. Of particular interest is the identification of additional tests of either geosphere or engineering components of the system that may be necessary to enhance the confidence in the predictions. Additionally, the identification of the benefits of various design alternatives that could be employed to delay, reduce or mitigate any radionuclide releases from the engineered barriers will aid in the development of the License Application design.

The TSPA-VA document itself will be quite lengthy. Recognizing that it can not be all things to all people, we will strive to provide capsule summaries of each major section for the reader who does not care to see the details of the analyses, while providing adequate details in the main body to allow a technical specialist the opportunity to see the basis for the assumptions used in the analyses.

5.2.8 Conduct a Peer Review of the TSPA Assumptions, Results and Conclusion

The total system performance assessment for the Viability Assessment will be peer-reviewed. The objective of the TSPA-VA Peer Review is to provide a formal, independent evaluation and critique of the TSPA-VA for the Civilian Radioactive Waste Management System Management and Operating Contractor. The TSPA-VA Peer Review Panel is to consider not only the analytical approach, but also its traceability and transparency. The review of the analytical approach is to include an evaluation of: (1) the physical events and processes considered in the analyses, (2) the use of appropriate and relevant data, (3) the assumptions made, (4) the abstraction of process models into the total systems model, (5) the application of accepted analytical methods, and (6) the treatment of uncertainties. The review criteria include: (1) the validity of the basic assumptions, (2) alternative assumptions, (3) the appropriateness and limitations of methods and implementing documents, (4) the accuracy of the calculations, (5) the validity of the conclusions, and (6) the uncertainty in the results.

The TSPA-VA Peer Review was formally commenced in February 1997 and is expected to be completed by March 1999. The Peer Review has been divided into four phases: Phase 1 – TSPA Orientation, Phase 2 – Modeling, Scenarios and Abstractions, Phase 3 – Draft TSPA Review, and Phase 4 – Final TSPA Peer Review. Interim reports are scheduled to be completed following the first three phases of the review, and a final report concludes Phase 4. The goal of the interim reports is to provide timely input to the TSPA analysts to assure significant issues are not overlooked in the TSPA-VA. The initial interim report was completed in June 1997 (Whipple et al., 1997). The intent of the final Peer Review Report is to provide comments, concerns, conclusions and recommendations in order to support the development and conduct of the License Application TSPA.

5.3 TYPES OF MODEL ABSTRACTIONS TO BE USED IN TSPA-VA

"Abstraction" is defined as a process of capturing or simplifying very complex and multifaceted processes that occur over many spatial and temporal scales in a manner that permits the important aspects of the processes to be included in total-system performance calculations. Abstraction is an essential element of performance assessment because of computer and personnel resource limitations. In particular, probabilistic TSPA predictions require numerous computer simulations to create performance-measure distributions that adequately cover the range of possible outcomes. However, these numerous simulations would not be feasible with existing resources if conducted with detailed process-level models. Thus the need for simplification. (See Sections 7.1 and 7.2.)

The major types of model abstractions to be used in TSPA-VA include: (1) domain-based abstractions, (2) process-based abstractions, (3) dimensionality abstractions, and (4) response-surface abstractions. Each of these types of abstractions is briefly discussed below. Greater details specific to each process model are presented in the individual sections of Chapter 6, and a review of abstractions as the basis of the TSPA-VA model and code architecture is given in Section 7.2.

<u>Domain-based abstractions</u>. Because of gravity, there is a general flow of fluid in one direction in the potential repository, which allows for a more or less natural division of the spatial domain into a series of regions, each dominated by one or more physical-chemical processes. In the case of Yucca Mountain, the obvious decoupling in space is: the waste-form, the waste package, the emplacement drift and engineered materials surrounding the waste package, the unsaturated zone between the drift and the water table, the saturated zone, and the biosphere. Both energy and mass are transported downstream (i.e., with gravity) from domain to domain, but since the main goal of TSPA is to track and predict radionuclide mass transport from the waste-form domain to the biosphere domain, the main rationale of this spatial abstraction is based on the transport of mass from one domain to the next. Thus, there is a separate radionuclide transport model for each spatial domain, each run sequentially in the TSPA-VA code, with output-mass versus time from an upstream spatial domain serving as the input-mass versus time for the spatial domain immediately downstream.

<u>Process-based abstractions</u>. In addition to the decoupling in space of the transport models, there is another logical decoupling by physical-chemical process, for example, the decoupling of thermohydrologic and flow processes from transport processes. This is based on the assumption that the energy and entropy of the decoupled processes flows primarily in one direction. In particular, it is assumed that the thermohydrology (or just hydrology, after the thermal pulse decays) establishes

and controls the liquid flux field for the transport-based models, but that transport-induced processes, such as mineral precipitation, only weakly feed back to thermohydrology or hydrology. If we make the further assumption of steady-state flow, i.e., the parameters from the flow equations that appear in the transport equations are constant with time, then the thermohydrology and hydrology models can be solved first, followed by the transport models.

Dimensionality abstractions. In general, the process models are constructed to be fully three dimensional. Including this level of detail is believed necessary to capture all of the details of the flow and transport in geologic media. However, including this detail in TSPA predictions is not always necessary in that the dimensionality of the model may not significantly affect the predicted response from a performance perspective. Therefore, a range of dimensionality abstractions may be conducted, including:

- 1-D (vertical) models of drift-scale thermohydrology representing the 'center' and 'edge responses of the repository, abstracted from 2-D x-z or 3-D models.

- 2-D vertical cross-section flow and transport models at representative locations in the unsaturated zone (e.g., E-W or N-S transects through the center of the repository), abstracted from the overall 3-D site-scale flow and transport models.

- 1-D (horizontal) models of SZ transport representing multiple non-interacting streamtubes, abstracted from 3-D ambient flow/transport models.

- 2-D (vertical) models of liquid dripping onto the waste packages, abstracted from 3-D thermohydrology models.

Response-surface abstractions. Response surfaces (multidimensional tables of the key output parameter as a function of key input parameters) are the next level of abstraction, which require even less computational time within the probabilistic TSPA-VA model, but could require a great amount of computational time and resources prior to running the overall TSPA model, if it is determined that the response surfaces must be created with the highest dimensionality, most-detailed, process-level model. For instance, it may be true that proposed simple models (reduced dimensionality, simplified representation of processes, etc.) are inadequate. Perhaps they have so few measurable parameters, or the dimensionality and discretization have been reduced so much, that they cannot adequately predict system response over the supposed uncertainty range. Or perhaps they do not allow a high enough degree of coupling to other domain- and process-based abstracted models. In this case, the only possible abstraction or simplification alternative may be to develop response surfaces based on the complex model. Here we mean that the complex model is run relatively few times to develop a curve fit of the nonlinear system response as a function of time, space, and the key model input parameters. Then, the system response for other values of the input parameters is interpolated from the response function. (Ideally, extrapolation would never be attempted.) Consider the thermohydrology process model as an example. Temperature (T) and relative humidity (RH), which are the primary outputs (dependent variables) of the thermohydrology models could be determined as a function of uncertainties in material properties, conceptual model, and local fluid flux (q) by running several process-level calculations over the uncertainty ranges of these independent variables. The results could then be tabulated as a multidimensional table of T as a function of material properties, conceptual model (e.g., ECM vs. DKM), and liquid flux; and similarly for R.H.

5.4 TREATMENT OF UNCERTAINTY AND VARIABILITY IN TSPA-VA

An important consideration in any prediction of performance is the degree of confidence in that prediction. This aspect is important when evaluating any engineered structure or system. In the case of a radioactive waste repository, the confidence in the prediction is exacerbated by the long time frames of concern, the complex interactions of a range of different processes, and the natural variability in the engineered and geologic components of the system.

In general, three types of uncertainty exist and need to be addressed in the TSPA. These include conceptual model uncertainty, parameter uncertainty, and stochastic uncertainty. Conceptual model uncertainty relates to the physical-chemical model used to describe the process, an example being the conceptual model of unsaturated zone flow in a fractured-porous media as either an equivalent continuum model, a dual permeability model, or a discrete fracture model. Parameter uncertainty relates to the specific property values used to populate the model, an example being the matrix and fracture flow properties used in the unsaturated zone flow model, such as fracture and matrix permeability and the interconnection area between the fractures and matrix.[6] Stochastic uncertainty relates to the spatial and temporal randomness inherent in natural processes (this is usually referred to as variability or more precisely as the uncertainty in the variability), an example being the distribution of fracture and matrix properties over the scale of the unsaturated zone flow model.

Table 5.4-1 details the aspects of uncertainty and variability that are planned to be addressed within TSPA-VA. The first column indicates cases where parameter uncertainty is being addressed within the context of the process model. These correspond to the process-level sensitivity analyses referred to in Section 5.2.2 whose aim is to determine the key parameters that need to be carried forward into the TSPA analyses.

The second column in Table 5.4-1 indicates cases where uncertain parameters within the TSPA model itself will be evaluated. Commonly the key parameters within these models will be sampled from PDFs which characterize the uncertainty in these parameters. However, in some cases we expect to bin the uncertainty in the parameter into discrete probability groups (i.e., not use a continuous function, but discrete probabilities or histograms).

The third column in Table 5.4-1 indicates cases where conceptual model uncertainty will be evaluated within the TSPA analyses. Although it is desirable to "parameterize" conceptual model

[6] Making the distinction between model uncertainty and parameter uncertainty is somewhat artificial, since a model is in essence a product of its parameters, and a comprehensive enough model can usually encompass all of the postulated conceptual models through variations in its parameters.

uncertainty to the extent possible, in most cases this is not feasible. Therefore, generally we will conduct alternative realizations of the expected consequences using the reasonable range of alternative models to illustrate the effects of this uncertainty. In some cases we will weight the alternative models and present the combined results. (Although this approach is common, it tends to shift the discussion from the appropriateness of the conceptual model to the appropriateness of the weighting factors. Because we believe the key aspect is the appropriateness of the model, we will tend to show the individual conditional results rather than the weighted results—but see Section 7.3 for details on this topic.)

The fourth column in Table 5.4-1 indicates cases where parameter variability will be explicitly included in TSPA-VA. This variability is included to capture the heterogeneity in the geohydrologic and engineering components of the repository system. For example, the thicknesses of the individual lithologic units are not uniform from place to place across Yucca Mountain. In addition, the infiltration rate, percolation flux, and therefore seepage flux, vary from location to location. Variability in the thermal output of different waste packages combined with the variability in the percolation flux and the thermo-hydrologic characteristics of the rock mass around the drifts combine to yield a spatially variable thermohydrologic response which in turn leads to a variable thermochemical response. Finally, given that there are approximately 10,000 waste packages that would be manufactured over about a 40 year time period, we expect there to be variability in the material characteristics from waste package to waste package as well as some variability from location to location on a single waste package (for example near any welds). These variabilities will be included in every prediction of post-closure performance.

An important consideration when including spatially variable processes in TSPA analyses is how much discretization is necessary to capture the essence of the variability without overburdening the computational resources. For example, it is not feasible to simulate the thermohydrologic response in the vicinity of every waste package. Nor is it feasible to simulate the degradation of each of the 10,000 packages and the release of radionuclides from each individual waste package that has been breached.

The approach we have taken in previous TSPA analyses, and will continue in TSPA-VA, is to discretize the system into representative spatial groups for the key hydrologic, thermohydrologic and waste package degradation processes. Within a group, the flow or thermohydrologic response or waste-package degradation will be the same, but there is variability from group to group. For example, we intend to discretize the repository block into a small number of segments (six were used in TSPA-1995) where the average percolation flux may vary from segment to segment. We also intend to divide the repository into an inner and outer zone with the difference being the thermal response resulting from edge cooling effects. We also intend to divide the waste packages into about three groups corresponding to the heat output from the different thermal loadings (high heat output corresponding to commercial PWR fuels and low heat output corresponding to high-level waste glass). The degradation of the waste packages will be simulated with a representative number of packages (400 were used in TSPA-1995) and the results normalized to the entire number of packages. At present we have not determined the number of release points for unsaturated zone transport. Although the capability exists to utilize all 10,000 waste package locations, it is more feasible that a reduced number (say 100) will be used to capture the spatial transport heterogeneity in the unsaturated zone.

The inclusion of spatial variability in the TSPA analysis, although making the analysis more realistic, can make the results less transparent. If all waste packages were subject to the same environment and failed in exactly the same way at the same time, and all release modes and rates at all waste package locations were similar and the transport in the unsaturated and saturated zone was uniform, then relatively simple calculations could be performed. To the extent that such calculations are instructive and help the reader understand the basic elements in the analysis, we intend to include them in our documentation.

A detailed description is given in Section 7.3.4 regarding the type of uncertainty and variability to be included in TSPA-VA for each component model, and the way it will be incorporated in the analyses. Also, Sections 7.3.2 and 7.3.3 describe how uncertainty will be displayed in the final results as it affects the potential dose to future generations.

5.5 SUMMARY

The general approach to be employed in TSPA-VA is analogous to the approach followed in previous TSPA iterations for the Yucca Mountain repository system. The primary difference lies in the direct inclusion of process model results in the TSPA analyses and a direct linking of consistent parameter distributions across different process models. Although the inclusion of the process model results makes the link back to the process model (and therefore the fundamental understanding derived from laboratory and *in-situ* observations) more traceable, it adds to the complexity of the analysis.

Although our focus is on the VA defined objective of "probable behavior" of the Yucca Mountain repository system, a wide range of sensitivity and uncertainty analyses conducted with both the process models and the abstracted models used in TSPA will assist us in quantifying the degree of confidence in that assessment. An important use of these sensitivity analyses is to evaluate the contribution of different elements of the system, both site-related and engineering-related, to the overall performance. For example, if a very conservative assumption is made concerning one aspect of the system and the system is still able to adequately protect public health and safety for very long time periods then the confidence in decision makers is enhanced. In addition, these sensitivity and uncertainty analyses will aid in identifying the key site and design features that most significantly impact the probable performance. These analyses will aid in the evaluation of the potential benefits of alternative design options that may be used in the License Application.

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Table 5.4-1. Uncertainty and Variability to be Evaluated in TSPA-VA

Process Model	Parameter Uncertainty Evaluated in Process Model	Parameter Uncertainty Evaluated in TSPA-VA	Model Uncertainty Evaluated in TSPA-VA	Parameter Variability Included in TSPA-VA
Climate Model		✓		
Infiltration Model		✓	✓	✓
Site Scale UZ hydrology model	✓	✓	✓	✓
Repository-scale thermohydrology model	✓			✓
Drift-scale thermohydrology model	✓		✓	✓
Seepage model	✓	✓	✓	✓
Drift-scale thermochemical model			✓	+
Drift-scale thermomechanical model	✓			
Drift-scale coupled T-H-M-C model	✓			
Waste package degradation model	✓	✓	✓	✓++
Cladding degradation model	✓	✓	✓	✓++
Inventory				✓
Waste form degradation model			✓	✓++
Radionuclide mobilization model		✓		++
Drift-scale transport model	✓	✓		++
Site-scale UZ transport model	✓	✓		✓
Site-scale SZ flow model	✓	✓		
Site-scale SZ transport model	✓	✓		
Biosphere transport model		✓		
Volcanic effects model		✓	✓	
Tectonic effects model		✓		
Criticality effects model		✓		

\+ variability correlated to thermohydrologic variability

++ variability correlated to thermohydrologic and thermochemical variability

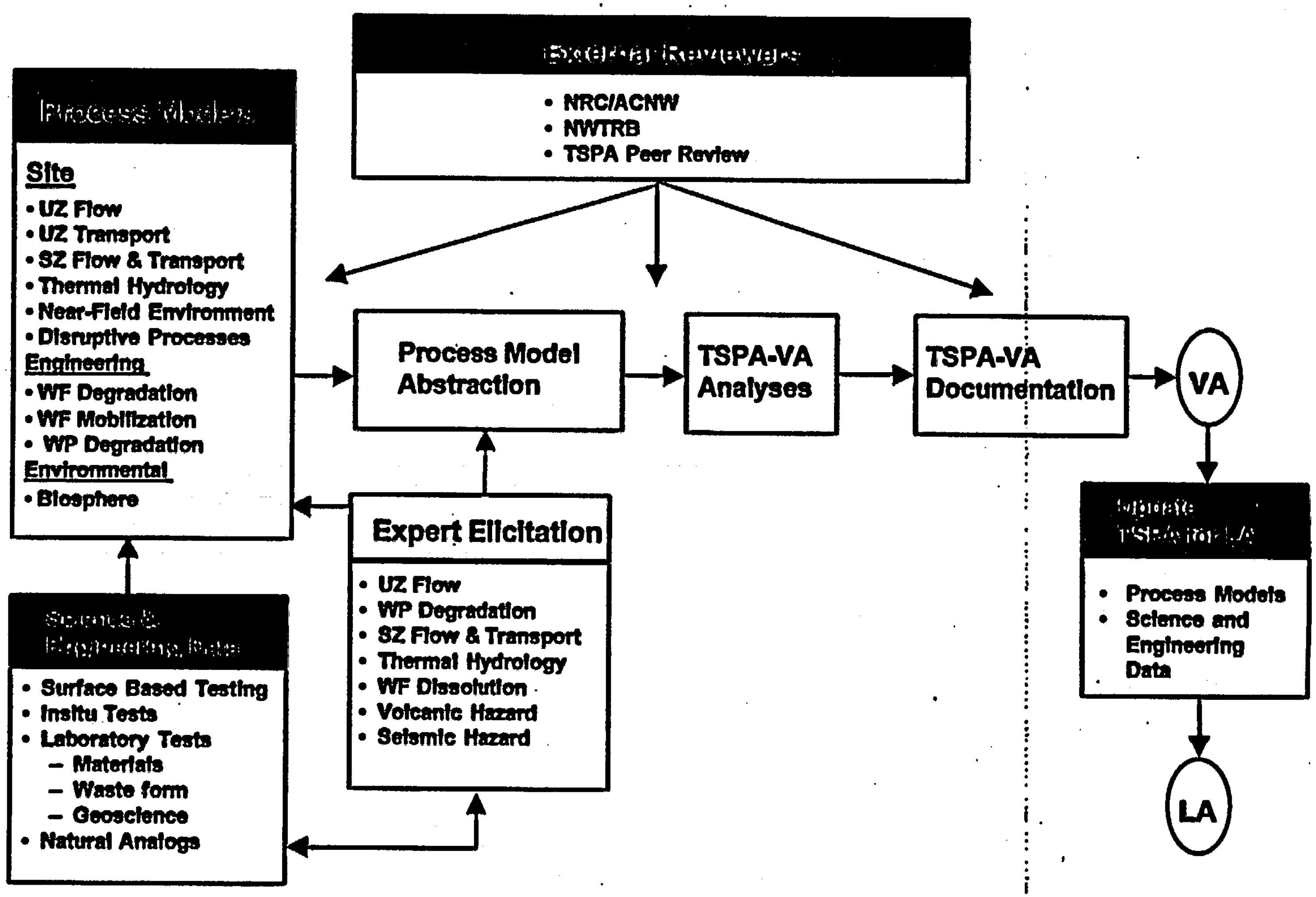

Figure 5.2-1. Development of Integrated TSPA-VA

6.0 SUMMARY OF MODEL ABSTRACTIONS IN TSPA-VA

6.1 UNSATURATED-ZONE FLOW

Mike L. Wilson, Susan J. Altman

6.1.1 Introduction

The "unsaturated zone" (UZ) is the portion of the geosphere where the rock pores and fractures are only partially filled with water. The UZ reaches from the ground surface down to the water table. (Below the water table is the "saturated zone," where the rock is completely filled with water. There can also be locally saturated regions, called perched-water zones, within the UZ.) The potential repository at Yucca Mountain would be in the unsaturated zone, approximately 350 meters above the water table. Unsaturated-zone water flow has long been considered one of the key processes to consider for Yucca Mountain performance assessment.

Past performance assessments (TSPA-1995: M&O, 1995; TSPA-1993: Andrews et al., 1994, and Wilson et al., 1994) have found calculated peak doses to be sensitive to (1) the present percolation rate at the potential repository horizon, (2) the amount of increase in the percolation rate under future wetter climate conditions, (3) the partitioning of flow between matrix and fractures, and (4) the amount of seepage into emplacement drifts. As will be discussed in succeeding subsections, the UZ-flow modeling for TSPA-VA is designed to explore these sensitivities further and to look for additional sensitivities that might affect performance results.

There are two primary outputs from the UZ-flow component: the mountain-scale UZ groundwater-flow field and the amount and distribution of seepage into emplacement drifts. Within the overall structure of TSPA-VA, UZ flow is closely related to all the other model components (except biosphere). UZ flow is clearly intimately connected to UZ thermohydrology (both mountain-scale and drift-scale) and UZ radionuclide transport. The seepage-into-drifts component of UZ flow is an important input to near-field geochemical environment, waste-package and drip-shield degradation, waste-form and cladding degradation, and engineered-barrier-system (EBS) transport. UZ flow is connected to saturated-zone (SZ) flow and transport through the water-table height and potentially through the amount of water crossing the UZ/SZ interface. Lastly, there is potential for disruptive events, especially volcanic and seismic events, to affect the UZ flow. Following is some elaboration on the connections between UZ flow and other TSPA-VA components.

UZ thermohydrology. Calculated UZ flow serves as an initial condition and far-field boundary condition for thermohydrology (TH) simulations. In practice, the stratigraphy and hydrologic parameters defined for the UZ flow are provided to TH modelers for input into their simulations. Mountain-scale TH calculations are used to modify the UZ flow during the thermal period.

hydrothermal conditions. Two problems with the Weeps model are (1) it ignores the rock matrix and thus any potential performance impact of flow in the matrix; (2) much of the data that it requires has not been collected and might be difficult (if even possible) to collect.

Another important flow model is the dual-permeability model (DKM), which has not been used for TSPA so far, but which has been used for other performance-assessment calculations (Altman et al., 1996). The DKM allows computation of flow in pressure disequilibrium in matrix and fracture continua, and appears to be a reasonable compromise between the ECM and Weeps models. However, it has its own problems, including (1) computational inefficiency and (2) lack of data describing the coupling term between matrix and fractures. The latest YMP UZ-flow model (Bodvarsson et al., 1997) uses a DKM formulation for UZ flow, and that is the formulation that has been selected for use in TSPA-VA. The DKM conceptual model has the flexibility to represent almost the entire range of possible flow behavior, since by altering its parameter values the predicted behavior can change continuously from the ECM (which is dominated by matrix flow) to flow almost entirely within the fracture network. Also, rivulet flow within the fractures can be captured by means of the fracture-matrix coupling parameter, which is discussed briefly below.

TSPA calculations of UZ flow up to now have primarily been done with only one spatial dimension (i.e., assuming strictly vertical flow). TSPA-1995 (M&O, 1995) included some evaluation of the 1-D assumption by comparison with a 2-D cross section taken out of the Lawrence Berkeley National Laboratory (LBNL) 3-D model (Wittwer et al., 1995). They found that the 1-D and 2-D calculations compared favorably, but it is important to note that the LBNL model did not yet include adjustments for perched water at that time. The current LBNL model (Bodvarsson et al., 1997) indicates significant nonvertical flow below the repository.

One of the key uncertainties in the UZ flow is in the upper boundary condition; specifically, the appropriate value for the mean percolation flux and its spatial and temporal variability. It is important to note that estimates of mean surface infiltration above the repository area have gone up significantly in the last two years, so the infiltration values used for TSPA-1993 (Wilson et al., 1994; Andrews et al., 1994) and TSPA-1995 (M&O, 1995) are much lower than those that will be used for TSPA-VA. So far, TSPAs have taken percolation to be spatially uniform. Temporal variability was included in TSPA-1993 and TSPA-1995. The temporal variability was idealized as a step function by Wilson et al. (1994) and as a triangular function by M&O (1995), in both cases with a period of 100,000 years (simulations were carried out to 1,000,000 years). Short-term variability has not yet been considered in TSPA. Note that TSPAs so far have only modeled flow from the repository down, so the model boundary condition has been percolation flux at the repository, not infiltration rate at the surface. Another potentially important temporal variation is the water-table height. In TSPA-1993 and TSPA-1995, water-table rises were assumed to have the same functional form as the percolation changes, i.e., either a step function or a triangular function with period of 100,000 years.

6.1.3 General Description of UZ-Flow Modeling

Current understanding of UZ flow in Yucca Mountain is a product of over ten years of field observations, laboratory experiments, and numerical modeling. The most important data come from several surface-based drill holes and from the Exploratory Studies Facility (ESF), which is an 8-km-long tunnel through Yucca Mountain. Considerable amounts of data are available on rock-matrix saturations, water potentials, and temperatures; on chemical composition and isotopic abundances of groundwater and mineral deposits; on air permeability and air-pressure fluctuations; on rock types and mineralogy; on fault locations and offsets; on fracture density and orientations; and on matrix permeability and saturation/desaturation parameters. In addition, there is information on the upper boundary condition (i.e., infiltration) from a series of weather stations and shallow drill holes instrumented with neutron probes, and there is information on climatic effects from a variety of paleoclimate studies and from analogues such as present-day Rainier Mesa.

The official Yucca Mountain Project model of UZ flow is being developed at LBNL by Bodvarsson and co-workers 1977. Their goal is to synthesize all of the available data into a coherent, predictive model of water and air flow in the unsaturated zone. It is important to understand, though, that as much data as we have on Yucca Mountain UZ flow, we do not have enough data to eliminate all uncertainty. Yucca Mountain is a large volume of rock, air, and water, with all the above information at only a limited number of locations. Another way to put this is that LBNL is developing a calibrated model of UZ flow, but there are not enough data to identify a unique calibrated model—it is possible to fit the available data with multiple calibrated models. One of the functions of performance assessment is to consider such uncertainties and show how they translate into uncertainties about repository performance (e.g., uncertainty about radiation dose to an individual living near Yucca Mountain some time in the future). Thus, much of the emphasis in the UZ-flow modeling for TSPA-VA is on uncertainties, alternative models, and reasonable ranges of parameters.

As mentioned earlier, the current LBNL UZ-flow model uses the dual-permeability formulation of fracture and matrix flow and interaction. This is a continuum formulation, with a matrix continuum, a fracture continuum, and an interaction between them that is proportional to the pressure difference at each spatial location. The numerical formulation of the model utilizes the TOUGH2 computer code (Pruess, 1991). Model calibration is done using an inverse method implemented in ITOUGH2 (Finsterle, 1993) to optimize the model parameters (matrix and fracture hydrologic properties for 22 hydrogeologic units). In the LBNL model (which is used as the base-case UZ-flow model for TSPA-VA), flow is mostly through fractures in the welded layers and mostly through the matrix in the non-zeolitized nonwelded layers. A new feature of the latest LBNL model (Bodvarsson et al., 1997) is that a fracture-matrix coupling parameter, related to the wetted area of contact between fractures and matrix in each hydrogeologic unit, is used as an inversion parameter as well. As mentioned above, it is important to note that spatially variable infiltration at the surface in the current model is considerably higher than values that were being used just two years ago. The higher infiltrations come from the latest Project infiltration model (Flint et al., 1996), which is based primarily on neutron-hole data. Infiltration is not allowed to vary in the ITOUGH2 inversions, but infiltration uncertainty is explored to some extent by performing multiple inversions, with the infiltration map multiplied by different factors. The increase in infiltration estimates has important implications for repository performance.

The Yucca Mountain Project recently conducted a UZ Flow Model Expert Elicitation, in which Project data and models were presented to a group of experts (mostly from outside of the Project) so that they could provide an evaluation of the work being done (M&O, 1997b). Particular emphasis was placed on estimates of surface infiltration and deep percolation; probability density functions (PDFs) of infiltration and percolation were elicited from each expert, and the individual PDFs plus a mean PDF are presented in the report. This expert opinion is a useful supplement to the models that have been developed within the YMP. Some of the expert-elicitation recommendations have already been incorporated in the latest LBNL model (Bodvarsson et al., 1997), and the experts' probability estimates regarding infiltration will be used directly in TSPA-VA.

6.1.4 Important Issues

As part of the preparation for TSPA-VA, a three-day UZ-flow workshop was held on December 11–13, 1996. Much of the time in the workshop was spent discussing the current state of knowledge of UZ flow in Yucca Mountain and what the important issues are. A list of these issues was compiled by the participants (who included a broad cross-section of data gatherers, process modelers, PA subsystem modelers, and TSPA modelers from within the Yucca Mountain Project), followed by discussion of priorities and approaches to dealing with the issues in TSPA-VA. A complete description of the workshop and its results may be found in M&O (1997a).

The important issues were separated into four categories as shown in Table 6.1-1.

In addition to those issues in the table, some issues were considered to cut across the categories. Cutting across categories 1 and 2 were the following:

Do we need to include grid-scale heterogeneity?

- Should subgridblock-scale fractures be lumped with the matrix?
- How should we upscale matrix properties?
- How should we propagate uncertainty in upscaling?
- How should we include spatial variability in the parameters?

Cutting across categories 2 and 3 was:

What is the appropriateness of transient versus steady-state modeling?

Some issues were identified that involved modifications to the flow system because of repository heating. These issues are listed below, but are being considered under UZ thermohydrology rather than under UZ flow.

- What are the potential impacts of hydrothermal alteration on lateral flow?
- How do thermal perturbations affect perching?
- How do thermal/mechanical effects change channeling and seepage?
- Can we do time-dependent TSPA calculations? Do we need different models for "cool" vs. "hot" periods?

Similarly, the issue of water-table fluctuations with climate was deferred to the SZ-flow group.

There was also an integration issue: "How do we deal with different models for thermohydrology, flow, and transport?" Resolution of this issue has required close cooperation among the UZ-flow, UZ-thermohydrology, and UZ-radionuclide-transport groups.

The issues listed above are almost all being considered in TSPA-VA to some extent. However, two of the issues require field or laboratory experiments and are thus beyond the workscope of TSPA. These issues are "How representative are the isotopic and water-chemistry data?" and "What features, processes, and parameters affect fracture/matrix interactions (coatings, connectivity, aperture, flux, etc.)?" Addressing these issues would add to the defensibility of the TSPA calculations. For now, we have to assume that the measured isotopic abundances and water chemistry are representative of the system. Clearly, if this assumption is not true, the interpretations of the system could change profoundly, which could have a strong effect on the TSPA calculations. Fracture-matrix interactions are being addressed through numerical studies: sensitivity studies are being performed to assess different conceptual models of interactions between fractures and matrix and their effects. To ground these sensitivity studies with laboratory experiments would add strength to the models. Until these experiments are run, analysts have to assume that what is learned from the numerical studies adequately represents the physical system.

Another list of important UZ-flow issues has been generated (Barr et al., 1995), as part of a larger project to catalog features, events, and processes (FEPs) that are important to performance of a Yucca Mountain repository. The correspondence between the nominal-flow FEPs and the important issues listed above is not transparent for two reasons. First, UZ-flow as defined for TSPA-VA is only a subset of the "nominal" FEPs, which include thermohydrologic and surface-runoff processes, for example. Second, the lists are at different levels of detail; the list above contains many rather specific modeling issues, for example, whereas the FEP "trees" are more general. We believe that all purely UZ-flow FEPs are being captured in TSPA-VA, either explicitly or implicitly.

Many of the above issues are being addressed by the current field-testing program, although only a few of the planned tests will have results that are timely enough for use in TSPA-VA. Some of these are briefly described below.

Niche studies are currently being carried out to investigate seepage into drifts. These studies evaluate ambient seepage by closing off niches in the ESF and monitoring inflow of water (if any) and changes in hydrological conditions in the walls of the niches. Active water and tracer tests are also being conducted, with water and tracers being introduced above the niches. The results of the active tests will hopefully provide seepage rate as a function of the total introduced percolation rate, which could be used directly to help calibrate the model for seepage into drifts.

Various PTn studies are being conducted to evaluate the potential for lateral flow within the PTn and to evaluate the effects of faults intersecting the PTn. These studies are being conducted in both the North Ramp and the South Ramp and include detailed matrix-parameter evaluations from measurements on cores from short boreholes, and measurements of moisture tension close to faults. Data from these tests are currently coming in and are being evaluated.

Additional isotope and fracture-coating studies are ongoing, with new data being obtained from the South Ramp of the ESF tunnel. Isotopic data such as ^{36}Cl and tritium measurements will expand our knowledge of fast pathways through the PTn, and fracture-coating age measurements will provide information on the hydrological and geochemical histories of individual fractures and fracture zones. Tests are planned to evaluate percolation flux, seepage into drifts in different geological media, the fracture-matrix flow components of the PTn and its role in buffering episodic pulses, fracture-matrix interaction, etc.; data from these will be available for TSPA-LA, but not for TSPA-VA.

6.1.5 Major Assumptions and Abstraction Approach

Major assumptions. The major UZ-flow assumption for TSPA-VA is that the LBNL model (Bodvarsson et al., 1997) is an adequate representation of flow in Yucca Mountain. We will consider variations in model parameters, but only within the dual-permeability model. Following is a list of the major assumptions for our approach. Note that nearly all of these major assumptions are being tested in sensitivity analyses (see analysis plans in M&O,1997a).

- Dual-permeability flow modeling (i.e., coupled matrix and fracture continua) is adequate. The dual-permeability model is capable of representing a large range of potential UZ-flow behaviors: fracture-matrix interaction, fracture and flow-channel spacing and geometry, effective fracture apertures, and fracture- and matrix-flow velocities all vary greatly as the model parameters vary. In future work, alternative models of the sort discussed in Chapter 24 of Bodvarsson et al. (e.g., discrete fractures, fractal fractures, etc.) should be evaluated as well, but they are not considered for TSPA-VA.
- Steady-state flow modeling is adequate. Climate changes will be included by using a series of steady states; because of that, the flow could be said to be quasi-steady state

rather than steady state. Perturbations to flow caused by repository heating might also be included by means of a series of steady-state flows, with the flow perturbation modeled by multipliers to the ambient UZ flow, as described briefly in Section 6.2.5. Such thermohydrologic perturbations will probably be considered only in sensitivity cases, because the waste packages are expected to last through the period when flow is strongly perturbed.

- Matrix hydraulic properties used are within the range of laboratory measurements, but in some cases adjusted to get better fits to matrix-saturation measurements or other data.
- Fracture hydraulic properties are based on air permeabilities, fracture frequencies, and fracture orientations measured in drill holes and in the ESF. In some cases, the inferred fracture properties are adjusted significantly in order to get better fits to matrix-saturation measurements or other data.
- The van Genuchten/Mualem functional form is satisfactory for use to represent the saturation/desaturation behavior of both matrix and fractures.
- The fracture-matrix connection area (i.e., area available for flow between fractures and matrix) is reduced below the geometric area implied by the fracture spacings used. Physically, this reduction represents effects of channelization of flow in fractures. The amount of reduction is chosen to optimize the fit to matrix-saturation measurements or other data.
- Small-scale heterogeneity does not need to be included (hydrogeologic units are homogeneous).
- Infiltration at the surface is spatially variable, with the variability given by Flint et al. (1996). Sensitivity to infiltration is investigated by multiplying the infiltration distribution by a constant factor, keeping the same spatial variability. We might also include a sensitivity case in which different assumptions are made about the spatial variability (based on suggestions made during the UZ Flow Model Expert Elicitation; M&O, 1997b).
- The lower boundary of the model is at the water table, which is fixed by drill-hole observations. For future climates, the water-table rise will be determined by saturated-zone modeling.

In addition to the mountain-scale UZ flow to which the above assumptions primarily apply, we need a model for seepage of water into emplacement drifts. There are additional assumptions for the seepage model:

We assume that seepage into drifts can be expressed as a function of the far-field flow in the vicinity of a drift. The functional relation may be probabilistic, especially in estimating how many waste packages are contacted by seepage.

Abstraction approach. The preferred abstraction approach is simply to use the LBNL process model directly (i.e., no abstraction). It was initially expected that the model would be simplified, probably by reduction to 2-D or even 1-D. However, the process modelers and site-characterization data gatherers have strongly recommended that 3-D is important to represent Yucca

Mountain flow adequately. This recommendation is based primarily on the flow below the potential repository, where there is thought to be significant nonvertical flow because of heterogeneity in the locations of the zeolitic layers and perched water. There are plans to make some comparisons with reduced-dimension models, but the rest of this discussion assumes that the 3-D UZ-flow model is used directly for the TSPA simulations.

There would be two ways to transfer the UZ-flow results to the UZ-radionuclide-transport model, which has been chosen to be the particle-tracking method in the computer program FEHM (LANL, 1997): (a) use the UZ flow fields calculated by TOUGH2 directly as input to the FEHM particle tracker, or (b) take the stratigraphy and calibrated hydrologic parameters and use them as inputs to a combined flow and transport calculation within FEHM. The primary advantages of the first option are that preservation of the UZ-flow calibration is assured, and it is not necessary to recalculate the flow and recheck the calibration. The primary advantages of the second option are that the FEHM particle tracker is already set up to use flow fields calculated by FEHM (the first option requires development of a linking program to take TOUGH2 output and generate FEHM input), and there is additional flexibility to refine the computational grid to make the transport calculations more accurate. Some limited testing has been done to compare these options, and although they both appear to be viable, the advantages of the first option are thought to outweigh those of the second option. Thus, we are tentatively planning to use the first option (flow fields calculated with TOUGH2, radionuclide transport calculated with FEHM), with the second option as a fall-back if unexpected problems are encountered.

An important consequence of using a complex 3-D flow model is that the number of different cases that can be run is limited—by computer-processing time, but even more so by the time needed for analysts to make necessary adjustments by hand for each case (to ensure proper model calibration). With current methods, it may not be practical to automate the procedure, at least not within the time available for TSPA-VA. By picking our cases carefully, we can still encompass the range of uncertainty in UZ flow and obtain information about sensitivity of performance to key model parameters, but without as much resolution as we might like.

For seepage, the abstraction approach is not as straightforward. There are no data available to calibrate such a model to, so there is necessarily more uncertainty as to the appropriate model of seepage. One of the UZ-flow analysis plans (and one of the thermohydrology analysis plans) calls for drift-scale UZ-flow modeling to investigate the conditions under which water will seep into a drift, and the amount of seepage that might be expected. We plan to use those modeling results as well as past results from the Weeps model (M&O, 1996, Chapter 6) and some conceptual ideas for estimating weep spacings from the mountain-scale dual-permeability formulation to define a "response surface" abstraction for seepage. The desired outputs of the seepage model are the fraction of waste packages contacted by seeps and the range or distribution of seep flow rates, both of which will vary with time because of thermal effects and because of climate change. It is anticipated that the outputs will be calculated as functions of the local fracture flux and perhaps some of the fracture hydraulic properties and/or the fracture-matrix connection area.

Abstraction testing. If the LBNL process model is used directly, there is no need for testing of abstractions against the process model. The models are tested directly against the data as part of the calibration procedure (i.e., each case must be calibrated).

For the seepage model, abstraction testing will consist of ensuring that the model is consistent with any drift-scale-modeling results that are available. Drift-scale modeling of seepage is currently being done both for ambient conditions and for TH conditions including repository heating. These drift-scale models include geostatistically defined small- to intermediate-scale variability in hydrologic properties. In addition, as mentioned above, it is possible that there will be some experimental results available in time for VA from ESF niche tests designed to study seepage of introduced water into excavated openings.

6.1.6 Base Case and Sensitivity Cases

The "base case" UZ flow for TSPA-VA is essentially the base-case LBNL UZ-flow model of Bodvarsson et al. (1997), plus some parameter variations. The parameter variations are not fully defined at this time, but they are expected to include three to five infiltration values (actually, three to five spatially variable infiltration maps) and possibly some limited variation of key hydrologic parameters (see discussion below) within ranges that would not adversely affect the model calibration. The mean probability distribution function for infiltration that was developed as part of the UZ Flow Model Expert Elicitation (M&O, 1997b), will be used to weight the results for different infiltration values. (This PDF indicates a great deal of uncertainty about estimates of present-day flux, with 1 mm/yr at 5% probability, 7 mm/yr at 50% probability, and 30 mm/yr at 95% probability.)

The base case will also include climate changes by means of putting together a series of steady-state flows. For a given realization, infiltration and water-table height would change from one steady state to the next, but the hydrologic parameters would not. Currently, we are considering building the climate scenarios from three climate states: present conditions (dry climate, mean infiltration approximately 5 mm/yr), the "long-term average" climate (infiltration on the order of three to four times present), and "super pluvial" (infiltration possibly as much as twenty times present). The appropriate infiltration increases and the timing of the climate changes are still being developed and are obviously quite uncertain. They will be based primarily on paleoclimate information.

The choice of sensitivity cases to be considered in TSPA-VA is subject to change as additional information becomes available, but currently two "alternative models" are envisioned:

- From parameter-sensitivity results reported by Bodvarsson et al. (1997) and from additional sensitivity studies that have been done, the key UZ-flow parameters are the infiltration, the fracture-matrix connection-area reduction factor, and the fracture van Genuchten alpha parameter. Also potentially important are matrix and fracture permeabilities, and the fracture van Genuchten *m* parameter (plus, for transport and possibly for thermohydrology, the fracture porosity), but these parameters appear to be less important than the first three above.

In order to explore more systematically the dependence of repository performance on the UZ-flow parameters, we define an "alternative" UZ model by using measured and inferred values for all matrix and fracture hydraulic properties (as opposed to the optimized values obtained from the ITOUGH2 inversion procedure) except for the fracture alpha parameter. Ranges will be defined for infiltration and fracture alpha, and they will be sampled from those ranges (the number of samples depending on how long each one takes to set up and run). For each sampled combination, the fracture-matrix reduction factor (*fmx*) will be optimized using ITOUGH2 to obtain a reasonable fit to the data. (A more efficient method would be to develop a response surface of *fmx* as a function of infiltration and fracture alpha using as few points as necessary, and then use this functional relation during the sampling instead of having to go through the inversion process for each sample realization.)

- We would like to define an alternative UZ-flow model that is similar in behavior to the Weeps model, which was used in TSPA-1991 (Barnard et al., 1992) and TSPA-1993 (Wilson et al., 1994). It is thought that this can be accomplished by using measured and inferred values for all matrix and fracture hydraulic properties, as in the first alternative above (but including fracture alpha as well), and setting the fracture-matrix reduction factor *fmx* equal to upstream relative permeability (there is some discussion of this choice for *fmx* in Bodvarsson et al., 1997). If the fit to matrix-saturation data is not sufficiently good with this simple choice, the *fmx* value would be scaled up or down to get a reasonable fit to the data.

There are two aspects of this alternative model that could provide useful insights into repository performance. First, this model has fracture-dominated flow everywhere, including the nonwelded layers, so it will show whether repository performance is adversely affected by a much greater fast-flow component than exists in the base-case model. Second, having *fmx* as a dynamical variable that depends on the flow, rather than as a fixed factor, could lead to differences in behavior when climate changes (and during the thermal period in thermohydrological models).

The model of seepage into drifts is not well enough defined at this time to know whether there will be only one model or whether there will be alternative models. Because there is much uncertainty about seepage (since we have no field data on which to base the model), it is likely that we will either have alternative models or wide parameter ranges in a single model in order to encompass the uncertainty.

The above "sensitivity cases" are the key cases, for which total-system performance will be analyzed. In addition, many sensitivity analyses are being carried out to test the various model assumptions and sensitivities, and to help define the parameters or ranges of parameters to be used in the total-system cases. These latter sensitivity analyses are described in M&O (1997a) and examine the behavior of just the UZ-flow subsystem rather than the total system.

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Table 6.1-1. Important Issues from UZ Flow Workshop

Category	Issues
1. Lateral flow and perched water below the repository	What is the appropriate dimensionality to use to model lateral flow for TSPA? Do we need to model UZ flow for TSPA in 3D, 2D, and/or ID? What is the extent of the perched-water bodies? How do the properties of the zeolites affect lateral flow? How do we use perched water for calibration?
2. Flow channeling and seepage into drifts	What are the representative multiphase characteristics for fractures (coatings, aperture distributions)? Are bulk permeabilities representative? - What is the spatial heterogeneity of fractures? - Are other fracture properties related to bulk permeability? What is the appropriate conceptual model for fracture flow? How do fracture/matrix properties affect seeps and channeling? How do spatial, temporal, and volumetric flux differences influence seepage into drifts? How do different conceptual flow models affect seepage and channeling? How representative are the isotopic and water-chemistry data? Does lateral flow in the PTn contribute to focusing flow? What features, processes, and parameters affect fracture/matrix interactions (coatings, connectivity, aperture, flux, etc.)? Can we incorporate what we know about fracture/matrix interactions into a continuum model?
3. Infiltration and future climate	What is the temporal variation of infiltration? How should we incorporate climate change? What is the range of present infiltration values? What spatial resolution is needed to properly represent variations in infiltration?

Table 6.1-1. Important Issues from UZ Flow Workshop (continued)

Category	Issues
4. Model calibration	What is the appropriate approach for model calibration? - How should we deal with non-unique calibration? - Should we "calibrate" or "bound"? (Is the answer different for different parameters?) Should faults be part of calibration? What is the applicability and robustness of available data to calibration (e.g., temperature, ^{36}Cl)? - How much should "inverse modeled" data be used vs. "lab modeled" data? How should we use perched water for calibration?

6.2 UNSATURATED-ZONE THERMOHYDROLOGY

Nicholas D. Francis, Mike L. Wilson, Cliff K. Ho

6.2.1 Introduction

Unsaturated-Zone (UZ) thermohydrology (TH) models are required for TSPA in order to provide an assessment of the potential impacts of repository decay heat on the natural geologic system. This includes an explicit determination of heat-driven processes occurring in both the far field (processes occurring at the scale of the mountain) and the near field (processes occurring at the scale of the drift). The potential repository horizon, located in the unsaturated zone at Yucca Mountain, contains in situ pore liquid water (and gas) that will react to the emplacement of heat-generating radioactive wastes. Energy will flow through the mountain from the repository by conduction and advection heat-transfer processes. Resulting phase-change processes driven by repository heating will allow the formation of dry-out and condensate zones with subsequent transport of water vapor and latent heat. These resulting processes will be played out for many thousands of years after waste emplacement. Subsequently, the repository-heat-driven processes will produce changes in the ambient hydrology and flow conditions of the mountain. Also, it is reasonable to assume that the current (ambient) hydrologic-property description of the mountain will probably be permanently altered as a result of the emplacement of heat-generating wastes. UZ-TH models provide the tools to make judgments as to the extent of thermally driven alterations to the natural geologic system.

The emplacement of radioactive wastes will influence local conditions around the waste package (WP) and within the drift. The thermodynamic environment in the emplacement drift is strongly dependent on the decay-heat characteristics from each of the individual waste packages. Quantification of the thermodynamic environment within the drift provides a description of conditions in the drift (e.g., hot, dry, humid, etc.) and surrounding the waste packages. The resulting conditions in the drift contribute to the performance of the repository by influencing the overall lifetime of the waste packages.

The emplacement of heat-generating wastes will also alter large-scale fluid and heat processes associated with the scale of the mountain. Heat-driven features at this scale potentially include the development of large-scale gas-phase convection cells and thermally altered liquid-phase flow fields both above and below the potential repository. Regions of dry-out formation with associated condensate drainage may occur on a large scale. The determination of the liquid-phase flow field (and how it is thermally altered) below the repository during the thermal perturbation is necessary for a complete description of radionuclide transport from the repository to the saturated zone (SZ)

UZ-TH results will serve as inputs to both near-field and far-field models used in TSPA-VA. TH results will provide relative humidity, air mass fraction, and gas-phase flow rate in the drift; temperature of the waste package (surface and center); and liquid saturation and temperature of the concrete liner and invert. This drift-specific information will be used by near-field models for waste-package and drip-shield degradation, waste-form and cladding degradation, engineered-barrier-system (EBS) transport, and near-field geochemical environment. TH results will also provide liquid-phase flow fields below the repository during the thermal perturbation. The far-field information can be used to account for the effects of the thermal disturbance during the radionuclide-transport calculations. Lastly, TH results, in combination with UZ-flow results, will be used to develop a model of seepage into emplacement drifts, which will be used by the near-field models.

Inputs to TH modeling will come from the UZ-flow, SZ-flow, and disruptive-events components of TSPA-VA. The hydrologic parameters are being defined within the UZ-flow task. Climate information is being defined within the UZ-flow (infiltration over time) and SZ-flow (water-table height over time) tasks. Rockfall information is being defined within the disruptive-events task. (Rockfall because of thermal-mechanical and seismic stresses will effectively add backfill to the emplacement drifts within hundreds to perhaps a thousand years, thus changing the thermal and hydraulic properties of the drifts.)

6.2.2 Previous TSPAs

For TSPA-1995 (M&O, 1995), two-dimensional drift-scale TH calculations were performed for two different thermal loads (25 and 83 MTU/acre), using the equivalent-continuum model (ECM) for heat and fluid flow. Infiltration rates of 0.05 and 0.3 mm/yr were modeled, for a homogeneous layered system. The model domain was a column within the unsaturated zone from the ground surface to the top of the water table, and from the drift center line to the center line between drifts. This results in a periodic model domain representative of the center of the repository. Cases with and without backfill were modeled. For cases with backfill, drifts were assumed to be backfilled using gravel with thermal conductivity of 0.6 W/mK, 100 years after waste emplacement. For nonbackfilled drifts, radiant heat-transfer effects were modeled explicitly. Because of the periodic boundary conditions, the modeled repository was effectively infinite in extent. A scaling concept was introduced to simulate a waste package located near the edge of the repository, but the scaling concept was not actually used for the TSPA calculations. WP temperatures and relative humidities over time were derived from the TH calculations and used for modeling waste-package and waste-form degradation.

For TSPA-1993, thermal calculations were performed using a conduction-only model (Wilson et al., 1994). Three-dimensional drift-scale and mountain-scale calculations were performed for two thermal loads (57 and 114 kW/acre). Effects on the hydrology (e.g., the extent of dry-out) were inferred from the extent and location of the boiling isotherm. For the drift-scale calculations, periodic boundary conditions were used (thus creating an effectively infinite repository) and drifts were assumed to be backfilled 75 years after waste emplacement using gravel with an effective thermal conductivity of 0.2 W/mK. Before backfill, radiant heat transfer in the empty drifts was approximated by thermal conduction with an effective thermal conductivity of 20 W/mK. The drift-scale calculations were used to represent early-time behavior. At late times (different for center or edge waste packages), an analytical solution was used instead of the periodic-cell model. This allows for reduced temperatures in response to finiteness of the repository. In the analytical-solution modeling, irregular waste streams and sequential emplacement of waste were also considered. WP temperature, dry-out volume, and fraction of dry waste packages, as functions of time, were derived from the thermal modeling and used for modeling seepage into drifts and waste-package and waste-form degradation.

6.2.3 General Description of UZ-Thermohydrology Modeling

The current understanding of UZ thermohydrology is not as advanced as the understanding of ambient UZ flow. Thermally driven effects have only recently been accounted for in TSPAs, and typically using some simplified format. However, the understanding of UZ thermohydrology continues to grow on an experimental level with the advent of the Exploratory Studies Facility (ESF) thermal-testing program. The thermal-testing program includes the small-scale single-heater test and the large-scale drift-scale test (see, e.g., Sobolik et al., 1996; Francis et al., 1997; Birkholzer and Tsang, 1996 and 1997; Buscheck et al., 1996 and 1997). Among other things, the thermal-testing program provides an opportunity for process-level conceptual-model validation and provides information on the coupled TH processes occurring as a result of heat input to the geologic setting. UZ-TH models at the scale of the mountain and drift have increased in complexity with increasingly more attention paid to physical details. With advances in computer technology, higher dimension numerical models are now possible for idealized conceptual flow models. Model dimensionality is an important consideration in the TH simulations of the potential repository.

Current drift-scale models (both TH and conduction-only) are typically specified as two- or three-dimensional (Wilson et al., 1994; Buscheck, 1996; M&O, 1995 and 1996b). Two-dimensional models are computationally very efficient, but they neglect important heat-transfer resistances associated with the finite areal size of a waste package (M&O, 1996a). Three-dimensional models explicitly account for the areal extent (i.e., the true surface area) of the waste package and do not neglect the resistance to heat transfer associated with the surface area of the heat generating source (refer to temperature comparisons made by Bahney, 1996, using conduction and radiation models). A comparison between TH models of different dimensions also indicates that important heat transfer processes are neglected by the lower-dimensional models (Baca and Brient, 1996). Three-dimensional models are recommended at this scale. The obvious drawback of the higher-dimensional drift-scale model is the reduction in computational efficiency. All of the drift-scale models mentioned above utilize the ECM conceptual flow model for heat and fluid flow in fractured porous media. This simplification is typically necessary to obtain reasonable computational times. TSPA-VA drift-scale TH models will make use of an alternative formulation of the ECM with a reduced matrix satiation value to ensure fracture flow of the liquid phase during the condensate-shedding periods.

Current mountain-scale models are typically specified as two- or three-dimensional (Buscheck and Nitao, 1993 and 1994; Pruess and Tsang, 1993; Ho et al., 1996; Francis et al., 1996). Most of these studies also utilize the ECM conceptual flow model for heat and fluid flow. Ho et al. (1996) considered a 2-D mountain-scale simulation including repository heating, using a dual-permeability model (DKM). This study indicates similar TH results when compared with the ECM simulations, with the notable exception of increased condensate shedding in the fractures during the repository heating and dry-out period. TSPA-VA mountain-scale TH models will make use of the alternative formulation of the ECM as well as applications of the DKM. The modified ECM can readily be used at the higher dimensions (2- and 3-D); use of the DKM will be restricted to mountain-scale TH simulations at lower dimensions (1- and 2-D).

6.2.4 Important Issues

A three-day UZ-thermohydrology workshop was held on January 21–23, 1997. A list of issues important to Yucca Mountain thermohydrology was compiled by the participants, followed by discussion of priorities and approaches to dealing with the issues in TSPA-VA. The key issues related to TH processes, as determined by the workshop participants, are listed in Table 6.2-1 as a function of major category considered during the workshop. These key issues were abstracted from a larger list of issues developed by the workshop core team and expanded by the participants during the workshop. Workshop participants included TSPA modelers, process-level modelers, waste-package and subsurface-repository designers, and site-characterization personnel. The importance of each issue was weighed against a set of criteria determined by the core team (and guided by previous NRC discussions as well as TH peer-review information) to be important to UZ-TH processes. The key issues, listed in order of importance in the table, were determined by the UZ-thermohydrology workshop participants. A complete listing of the issues and the methods used to prioritize them are given in detail in the Abstraction/Testing Workshop document, M&O (1997a).

The process issues important to TSPA-VA and related to thermohydrology are identified at the scale of the mountain as well as at the scale of the drift (see above). The key issues listed above form the basis for the development of the abstraction/testing analysis plans that resulted from the workshop activities. The workshop analysis plans resulted in specific tasks and sensitivity studies designed to address the development and thermal alteration of large-scale flow fields below the repository and the thermodynamic environment inside the drift after waste emplacement. Each of the required results is a function of model dimensionality, conceptual flow model (heat and mass), and the amount of alteration to the natural setting as a result of thermal stresses and chemical processes.

Issues related to model dimensionality occur at both scales considered in the resulting analysis plans. The issues are related to computational efficiency and the ability of a model to appropriately capture the physical phenomena associated with a process (M&O, 1996a).

Issues related to thermally driven alterations of the natural ambient state include changes to the fracture properties (primarily porosity and permeability) governing flow processes. Chemical or mechanical changes to the fracture properties influence the resulting gas-phase and liquid-phase flow fields predicted by the models (drift- and mountain-scale), and thereby potentially affect heat and radionuclide transport as well. Although the response of the mountain to these effects will not be fully coupled in the TSPA-VA analyses, simplifications that patch thermal-mechanical and/or thermal-chemical influences into a UZ-TH simulation have been proposed as a series of sensitivity studies.

Critical mountain-scale issues include the use of alternative conceptual flow models for both heat and fluid flow during the thermal transient. Of particular importance are the methods used to describe fluid flow in the fracture domain and transfer between fractures and matrix. Conceptual models that will be investigated include the dual-permeability model, which allows for pressure disequilibrium between fracture and matrix domains. The equivalent-continuum model, which assumes equilibrium between fractures and matrix, will also be included for completeness. A special version of the ECM that allows fracture liquid flow to occur at matrix saturations less than one will be used for comparison to DKM and for thermal-load scaling studies performed at the mountain scale and used as input to drift-scale models. This weak form of coupling between mountain-scale models and drift-scale models will serve as the basis for determining repository "edge" conditions to be applied in the near-field models.

Drift-scale UZ-TH models are used to obtain approximations of the thermodynamic environment within the emplacement drifts and at the waste packages. This WP- and drift-specific information drives the evolution of the drift and EBS over time. The required information includes WP temperature (centerline and surface), relative humidity at the surface of the waste package, and air mass fraction in the drift. Other important thermal and hydrologic information at the scale of the drift includes the liquid saturations and temperatures in the invert materials and the concrete liner of the drift wall. In addition to the thermodynamic state variables, flow-rate information such as gas-phase flow rates in the emplacement drifts and the pervasiveness and rate of water dripping into the drifts are also very important to the performance of the EBS. All of this information is dependent on the conceptual flow model assumed in the simulations.

It would be desirable to make comparisons of different conceptual flow models at the drift scale as well as at the mountain scale, but 3-D DKM thermohydrology models are not feasible with current computers and programs. It is expected that the flow-model assumptions would have a significant effect on seepage into drifts and gas-phase flow rate and air mass fraction in the drifts, so those items of information will be obtained primarily from the 2-D mountain-scale modeling, where it should be possible to use the DKM for at least some of the simulations. (For gas-phase flow rate and air mass fraction, it is also important to use mountain-scale simulations in order to take into account possible effects of large-scale gas-phase convection.) The use of 3-D drift-scale models is critical for obtaining appropriate near-field temperatures and relative humidities, and fortunately it is expected that they are less sensitive to the flow-model assumptions. Detailed justification of these expectations will have to be left to future work.

6.2.5 Major Assumptions and Abstraction Approach

Major assumptions. The conceptual model governing heat and fluid flow is a key aspect of the model analyses and sensitivities studies. The amount and form of fracture flow, in particular, are very uncertain, and very important to some of the results. As noted by Baca and Brient (1996), it is important to use a model that allows for appropriate amounts of fracture flow. However, The choice of conceptual flow model is severely limited by computational-efficiency issues. The DKM has been selected as the preferred conceptualization of flow for TSPA-VA (see Section 6.1), but with current computational capabilities DKM is only practical for 1-D or 2-D models. (And even 2-D can be problematical.) As discussed earlier, 1-D and 2-D TH simulations can be acceptable at the mountain scale, but 3-D is necessary to obtain acceptable drift-scale results. Thus, drift-scale TH models (3-D) will use a modified version of the ECM conceptualization that has matrix satiation less than 1. Mountain-scale models will be primarily 2-D. If practical, the mountain-scale models will use DKM; if DKM is too slow for 2-D mountain-scale models, the modified ECM will be used for most calculations, supplemented by 1-D and 2-D DKM calculations. The modified ECM will be compared to DKM for some representative mountain-scale calculations in order to evaluate its accuracy.

It is assumed that waste packages situated near the repository "center" can be modeled with a typical periodic "unit cell" drift-scale model. It is assumed that waste packages situated near the repository "edge" can be modeled similarly, but with scaled thermal outputs, as described in Chapter 4 of M&O (1995). The heat-output scaling factor for the edge representation will be developed using a solution-matching technique that will reproduce the edge results from a 2-D mountain-scale model with nominal thermal load at the center of a 2-D mountain-scale model with lower thermal load.

Tom Buscheck and his co-workers at Lawrence Livermore National Laboratory are pursuing an alternative, more accurate, method of coupling drift-scale and mountain-scale TH models. Near-field TH results at different repository locations (e.g., "center" and "edge") can be computed using a combination of mountain-scale and drift-scale TH and conduction-only models in order to develop relationships governing the temperature, relative humidity, and air mass fraction at the drift wall and inside the drift at the waste package for different repository locations. The governing state-variable relationships at the drift wall and waste package are obtained from a hierarchy of models of different complexities; see M&O (1997a, Section 4.2) for details of this method. If available (and practical) in time for TSPA-VA, this method will be used instead of the scaling method described in the previous paragraph.

As for UZ flow (Section 6.1), small-scale heterogeneities are not included in the TH calculations for TSPA-VA, with the exception of detailed drift-scale calculations that are being done for the purpose of understanding seepage into drifts. Heterogeneity is thought to be essential for modeling seepage, but less important for the other TH quantities. Comparison of the heterogeneous calculations with nonheterogeneous ones will provide information as to the importance of small-scale heterogeneities.

Variability of thermal output among waste packages is included to a limited extent in the drift-scale calculations by including eight representative waste-package types. In the mountain-scale calculations, the thermal source is smeared, and has no spatial variability. Variation of thermal-output history across the repository because of sequential emplacement of waste over a period of years will not be considered. We assume that these approximations will provide an adequate range of thermal histories to represent repository behavior.

Another important assumption is that mechanical and chemical alterations of hydrologic properties (i.e., coupled THM and THC effects) can be neglected. This assumption is being tested by means of sensitivity studies; if these effects are found to be significant, they will be included in the TSPA-VA simulations in a simplified manner if possible (presumably by modifications of matrix and fracture permeability), but detailed inclusion would have to be left to future work (i.e., TSPA-LA). Some information on these effects should be available from the single-heater test in time for TSPA-VA; data from the drift-scale test will not be available until after TSPA-VA.

Abstraction approach. The anticipated form of the abstraction of UZ thermohydrology for incorporation into TSPA-VA simulations is a series of tables of far-field liquid-flow multipliers and specific near-field flow rates and thermodynamic state variables.

Mountain-scale TH calculations will provide the gas-phase flow rate and air mass fraction at representative "center" and "edge" repository locations. Mountain-scale calculations might also be used to provide liquid-phase flow-field multipliers for the thermal period at locations beneath the repository to the saturated zone. These multipliers would be used to approximately correct ambient UZ flow fields for TH effects (for example, fracture flux would be increased when there is condensate drainage or decreased during a dry-out period). The TOUGH2 computer program (Pruess, 1991) is being used for mountain-scale TH calculations.

Drift-scale TH calculations will provide temperature and relative humidity at the surface of the waste package, and liquid saturation and temperature in the invert and the drift liner. These quantities will be provided for two representative repository locations ("center" and "edge") and for different waste-package types. The drift-scale models include eight waste packages of differing heat outputs (representing both commercial spent fuel and defense high-level waste), but the TSPA calculations will probably only use three of them (a hot spent-fuel package, a medium spent-fuel package, and a "cool" high-level-waste package). The NUFT computer program (Nitao, 1996) is being used for drift-scale TH calculations.

Calculations of temperature within waste packages will be used to define the difference in temperature between waste-package surface and waste-package center as a function of time and waste-package type. This will then be added to the waste-package temperature from the drift-scale TH calculations to obtain temperature at waste-package center.

The abstraction approach for seepage into emplacement drifts was discussed in Section 6.1.5. We plan to take information from several sources (drift-scale UZ-flow and TH modeling, mountain-scale UZ-flow and TH modeling, past results from the Weeps model) and define a "response surface" abstraction for seepage. The desired outputs of the seepage model are the fraction of waste packages contacted by seeps and the range or distribution of seep flow rates, both of which will vary with time because of thermal effects and because of climate change. It is anticipated that the outputs will be calculated as functions of the local fracture flux and perhaps some of the fracture hydraulic properties and/or the fracture-matrix connection area. When temperatures are high, temperature may enter in as well because some of the seepage may evaporate.

Abstraction testing. Important abstraction assumptions that will be tested by sensitivity analyses include comparison of 2-D and 3-D results, comparison of DKM and modified-ECM results, comparison of open-drift results with radiative heat transfer to results with an effective-conductivity approximation, validity of the scaling approach for approximating "edge" effects, and comparison of mountain-scale TH flow fields to the approximated flow fields from the multiplier approach.

6.2.6 Base Case and Sensitivity Cases

The TSPA-VA "base case" for UZ-TH calculations will include information from subsurface-repository design, waste-package design, and site characterization. Subsurface design provides detailed design data related to the emplacement-drift geometry, total thermal load, and mode of waste-package emplacement. Waste-package design provides additional information related to waste-package placement strategy and fuel types as well as the base-case waste-stream information. Finally, site characterization provides the data related to geologic stratigraphy, hydrologic- and thermal-property data, infiltration rates applied at the ground surface, and climate change.

The base-case subsurface design is specified for an areal mass loading (AML) of 85 MTU/acre. This value remains constant in time. This mass-loading value includes only the commercial spent nuclear fuel (CSNF). The defense high-level waste (DHLW) and DOE spent nuclear fuel (DSNF) are simply placed in between CSNF packages (M&O, 1997c). However, their heat output is included in the TH calculations. The total amount of waste in the repository is 70,000 MTU, with 63,000 MTU in CSNF and 4,667 MTU in DHLW and 2,333 MTU in DSNF. The base-case emplacement-drift design is specified as a "point loading" thermal design without backfill. The waste packages are to be placed on-center inside the emplacement drift. The emplacement drift will contain a concrete liner and invert material (M&O, 1997b). The "point loading" repository design is described in general terms as CSNF waste packages spaced away from each other along the drift with emplacement-drift spacing similar to the CSNF-package spacing.

Waste-package design specifies the base-case waste-stream information as well as incorporation of the hotter "design basis" fuels for emplacement into the repository (M&O, 1997d). The design-basis fuels have much higher thermal outputs than the average waste package at the time of emplacement into the repository. Based on the decay characteristics of the base-case waste stream, the areal power density (APD) can be computed. The total initial APD is approximately 99 kW/acre, with 90 kW/acre in CSNF and 9 kW/acre in DHLW and DSNF. The APD is variable in time, depending on the decay characteristics of the individual waste-package types in the drift-scale models and of the average repository for the mountain-scale models. At this thermal load, only the upper (western) repository block will be required for waste disposal.

The base-case stratigraphy and hydrologic properties are obtained from the official UZ-flow model (Bodvarsson et al., 1997). In order to maintain consistency among all TSPA-VA models, the base-case properties and parameters developed in the UZ-flow task are applied to the TH models as well. Specifically, this includes detailed hydrologic-property data sets for fractures, matrix, and fracture-matrix interaction, and includes any parameter variability included in the UZ-flow base case (e.g., multiple infiltration assumptions). Thermal properties are obtained from a compilation of experimental results and models (Francis, 1997).

Although initial modeling is being done assuming constant boundary conditions, the base case for TSPA-VA includes climate change, which will be included in the TH models by means of step changes in the boundary conditions at specified times.

The TSPA-VA base case assumes that the emplacement drifts will remain intact for a period of hundreds to perhaps a thousand years, after which the drifts will be filled with rockfall rubble (Bhattacharyya, 1997). If practical, the change in the thermal properties of the drifts caused by this rubble will be taken into account in the base-case drift-scale TH models (unless it can be shown to have little effect).

Sensitivity cases for UZ thermohydrology include the UZ-flow sensitivity cases where meaningful (variations in fracture-matrix coupling cannot be analyzed if the modified ECM is used for TH calculations) and alternative repository designs.

Alternative repository designs of interest include inclusion of backfill and "line loading." The backfill material could be tuff gravel or quartz sand. The "line loading" repository design is described simply as waste containers spaced very closely along the drift, with emplacement drifts relatively far apart. Backfill is on the short list of preferred design options (see Section 4.1.1), so analysis of thermohydrology with backfill will definitely be included in TSPA-VA. Line loading is not one of the preferred options, but we expect to include at least some analysis of line loading as well.

Besides the above, additional design alternatives will be analyzed in support of the Yucca Mountain Environmental Impact Statement (EIS). For the EIS, two additional areal mass loadings are to be considered: 60 and 36 MTU/acre. Also, additional waste types and amounts will be considered for the EIS. In addition to the base case, with 70,000 MTU of waste, a case will be analyzed which includes all CSNF (estimated to be 105,000 MTU) and all DHLW and DOE SNF; additional cases will consider other types of waste as well, including DOE special performance-assessment-required waste, commercial greater-than-class-C waste, and plutonium surplus fissile materials.

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Table 6.2-1. Important Issues from UZ-Thermohydrology Workshop

Category	Issue
1. Thermohydrologic processes and parameters	What model should be used for fracture-matrix interactions in TSPA? How should fracture properties and thermohydrologic processes be upscaled? Do we need to include lateral (intra-unit) heterogeneity in TSPA?
2. Mountain-scale models	What alternatives for repository design should be considered in mountain-scale models? How important is the trade-off between 1-D/2-D modeling and 3-D modeling? How important is the dual-permeability model at the scale of the mountain? What is the impact of drift-scale-model coupling on the design of mountain-scale calculations?
3. Drift-scale models	Will variability of heat output among waste packages allow for condensate shedding onto cooler packages? How should seepage into drifts and onto waste packages under nonisothermal conditions be modeled? Is it necessary for TSPA-VA to provide drift-scale models that represent edge as well as repository-center conditions? Can we use 2-D drift-scale models or will 3-D models be required to accurately predict WP temperature and drift relative humidity?

Table 6.2-1. Important Issues from UZ-Thermohydrology Workshop (Continued)

Category	Issue
4. Coupled processes	Will phase-change processes cause chemical deposition and thus alteration of fracture and matrix properties? Will thermal stresses cause significant hydrologic-property alterations in regions of compression and tension? What effects would drift collapse have on WP temperature, RH in the drift, and seepage water contacting a waste package? Will evolution of a nonisothermal geochemical system have a significant impact on dissolved constituents that influence corrosion and solubility, speciation, and sorption of radionuclides?

6.3 NEAR FIELD GEOCHEMICAL ENVIRONMENT

David C. Sassani, S. David Sevougian

6.3.1 Introduction

General. The near-field geochemical environment is defined as the environment within the drift. The near-field geochemical environment (NFGE) model affects and is affected by all of the other processes (and associated models) within the engineered barrier system (EBS). As defined here, the NFGE model specifically focuses on major-element geochemistry within the potential emplacement drifts [see M&O (1997) for a discussion—the boundary of the NFGE model domain as defined in TSPA-VA is the drift wall], which includes the coupling to thermohydrologic processes. As discussed in Chapter 7, 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 amongst processes. This assumption is least tenable when applied to the near-field geochemical environment model, which is highly coupled and nonlinear, being influenced by thermal, hydrologic, and multi-component chemistry. This is evident by the numerous model interconnections shown in Figure 7.2-1.

Through its influence on the source term of radionuclides, i.e., through its influence on waste-package, waste-form degradation, and waste-form mobilization, the NFGE (as coupled to near-field thermohydrology) may be one of the most important models from an overall performance perspective. In previous TSPAs, the most important parameters were generally flow related, however, the reason for the general lack of importance of the NFGE may have been a lack of sophistication in the past NFGE models (see Section 6.3.2), rather than an intrinsic insignificance.

Input. Key inputs to the NFGE model include the major-element composition and thermodynamic/kinetic coefficients of the introduced in-drift materials, the thermohydrologic behavior of the entire repository, the gas-phase composition entering the drift through time, and the aqueous-phase composition entering the drift through time. These in turn depend to a large extent on the design of the repository: the thermal load, whether and what type of backfill is used, the waste-package material composition, the drift lining composition (e.g., concrete or steel), and also the far-field percolation flux, the reaction and reflux of condensate water, and the drift seepage flux. All these parameters will influence the predictions of the NFGE model.

Output. The output from the TSPA-VA NFGE model will be a set of major chemical compositional parameters over time and space within the EBS that are used by other EBS models. For example, if pH and carbonate concentration are the only parameters deemed important for waste-package or waste-form degradation, these will be the only outputs taken from the NFGE model (even though the model will predict many other species activities). In addition, the mineralogic description of EBS materials through time will be provided by the NFGE model for use in the EBS radionuclide transport model. The NFGE model will only be run for a certain number of introduced materials evolution scenarios with a finite number of incoming fluid compositions, i.e., for only a certain number of boundary conditions to the NFGE model. These include the following chemical compositions for the input boundary water and gas: J-13 water to thermally-perturbed water, and ambient pore gases to thermally-perturbed gases.

Connections to other TSPA-VA Components. Following is a discussion of how the NFGE model interfaces with other component models of TSPA-VA (from M&O, 1997):

Thermohydrology. The thermal disturbance due to repository heating affects the movement of water and gases throughout the mountain and within the potential emplacement drifts. This provides a number of the time-dependent boundary conditions for the NFGE, including the flux of groundwater and gas into the drift, and the in-drift temperature. The thermal effects can drive changes in the fluid and gas compositions through changes to temperature-dependent phase equilibria or reaction kinetics. Such compositional changes may also occur within the heated geosphere surrounding the EBS that can perturb the compositions of those incoming phases. The effects of thermal perturbations may also have long-term consequences relative to minerals and solids within the drift because of changes in phases stabilities and reaction rates. These effects can lead to changes in the behavior of waste-package degradation, the evolution/dissolution of the waste form, and both the hydrologic and transport properties of the engineered barrier system. These types of thermohydrologic changes to the near-field environment will affect the chemistry in the drift and may impact the rate and types of long-term radionuclide releases from the engineered barrier system into the geosphere. In addition, if mineral dissolution/precipitation processes are extensive enough, changes to the permeability/porosity in the near-field could feedback to the thermohydrologic processes, causing significant changes in liquid and gas movement.

Waste Package Degradation. The waste package degradation model defines the rate at which the various engineered barriers (inner and outer layers, etc.) of the waste package corrode, providing both the time of first penetration of the package and a time history of the number of breaches in the container. This provides the state of the waste package degradation through time, as well as the area of the waste package through which mass transport can take place. The in-drift geochemistry has significant impacts on corrosion of waste package barrier materials. For TSPA-VA, corrosion models will account for the effects of important geochemical conditions such as chloride concentration and pH. The composition of water contacting the waste package and the bulk oxidation state within the drifts will be supplied by the NFGE model. A specific NFGE submodel bounding the microbial contribution to the *bulk* chemistry will be coupled to the waste package degradation model via *localized* corrosion enhancements from microbial communities.

In addition, just as the waste package degradation will be affected by the fluid composition reacting with it, the waste package materials are an extensive mass of introduced materials. These materials and their solid corrosion products may exert controls on the aqueous and gas compositions in the drift, as well as provide a source of Fe-oxyhydroxy colloids, which can cause enhanced migration of certain radionuclides. The evolution of the waste package solid phases and their reactions with the aqueous and gas phases are integral parts of delineating the chemical conditions throughout the potential emplacement drifts.

Waste Form Degradation and EBS Transport. The waste-form degradation and EBS transport models define the rate of waste form reactions, the type and supply of mobile radionuclides at the waste-form surface, the radionuclide transport pathways and mechanisms through the engineered barrier system, and, ultimately, the radionuclide fluxes and types of mobile radionuclides delivered to the geosphere (at the edge of the EBS, i.e., the drift wall, which represents the "source term" for the geosphere models). The rates of degradation of the waste forms (including cladding) will depend upon compositional parameters of the gas phase and the aqueous phase reacting with the waste form. The mobilization rate through the geosphere depends on these parameters also, and depends upon the chemical interaction with the solid phases through which transport occurs. The NFGE model will provide the compositions of water and gas that may react with the waste forms and the state of materials through which radionuclide transport will occur. These aspects will consider the potential effects of corrosion of the waste package and the internal structural materials (e.g., basket tubes and guides made of carbon steel) and their corrosion products, in addition to those of cementitious materials within the potential drifts.

In addition, for TSPA-VA the waste-form degradation/mobilization models have been expanded to provide an input to the near-field geochemical environment tasks that includes the bulk water composition and the concentrations of colloidal radionuclide species of at the surface of the waste form (these parameters are in addition to the radionuclide composition of the aqueous phase). Given the large mass of waste form inside the packages, the resultant bulk water chemistry from reaction with the waste form may be very different from the starting fluid composition. Therefore, the waste forms themselves were identified as having potentially large geochemical effects. These resultant aqueous compositions represent a starting composition for reaction with the engineered materials through which the radionuclides migrate. Both the starting composition and the reaction with introduced materials will affect the bulk water composition that is passed from the near-field geochemical environment activities to both the unsaturated-zone transport and thermohydrology tasks.

Unsaturated Zone Radionuclide Transport. The unsaturated zone radionuclide transport (UZRT) model (Section 6.8) defines the movement of the radionuclides from the edge of the EBS, through the unsaturated zone, and to the start of the saturated zone. The main input from the NFGE model to the UZRT model is via the EBS transport model (Section 6.7), which provides the aqueous abundances of radionuclides at the edge of the engineered barrier system. However, the NFGE sensitivity studies on colloid transport (M&O, 1997) is being directly integrated with similar sensitivity studies for UZRT model in order to provide a fully integrated analysis of the potential for colloid transport to impact system performance. In addition, bulk composition of the aqueous fluid at the edge of the EBS is provided by the NFGE model to delineate the starting composition of the fluid migrating through the geosphere. The composition of this fluid can affect the ability of the system to retard dissolved radionuclides (through compositional effects on sorption coefficients) and may alter the existing lithologies.

Criticality. The criticality model will define the potential for the waste fissile materials to become configured such that nuclear criticality could occur, as well as the changes in source term and conditions resulting from a critical event. A portion of this work considers the possibility of such a configuration of fissile material being assembled within the drift (near-field) environment after release from waste packages (so-called "external" criticality). External criticality, therefore, is linked directly to radionuclide transport processes in the potential emplacement drifts and depends upon the temporal and spatial chemical changes that occur there. In addition, the conditional changes (mainly thermal) resulting from a critical event could affect the chemical environment within a drift.

6.3.2 Treatment in Previous TSPAs

Within the previous TSPAs (Wilson et al., 1994; Andrews et al., 1994; M&O, 1995), the near-field geochemical environment has been incorporated as a number of compositional variables within subsystem models, or implicitly within some of the ranges used for performance parameters (e.g., solubility-limited radionuclide concentrations). The most recent performance assessment modeling work (M&O, 1995) primarily employed the Repository Integration Program (RIP) (Golder, 1996). RIP is a TSPA code which contains a source-term model that analyzes waste-package degradation, waste-form degradation and mobilization, and transport of radionuclides through the engineered barrier system. It can utilize the NFGE model output parameters directly in the form of response surfaces or table lookups, which set the local environments of RIP "cells" representing various portions of the near-field, such as the waste form, the degraded package, and the invert. These compositional response surfaces can be used in RIP to affect waste-form degradation rates, as well as solubility-limited concentrations and equilibrium distribution of radionuclides amongst the phases (which would in turn affect the transport rate). These NFGE response surfaces could also be used within RIP to affect the waste-package degradation rate. (However, for TSPA-VA it is more likely that they will be fed directly to the external waste-package degradation model, WAPDEG, which generates first pit penetration rates and pit growth rates outside of RIP. Abstracted results of these simulations are then fed as additional response surfaces into the RIP package-failure module.)

The near-field geochemical environment implicitly included in previous TSPA calculations corresponds to the ambient water composition from Well J-13 and atmospheric oxygen and carbon dioxide fugacities. The impacts of pH variation and temperature variation have been incorporated *explicitly* into models of waste-package degradation, waste-form dissolution, and the solubility-limited concentrations of Np, Pu, and Am (M&O, 1995). A variable pH condition covering values of 6 to 9 (with 7 taken as the base-case) was incorporated *implicitly* into the distributions of solubility-limited concentrations to define the mobile radionuclide concentration. This range of pH reflects the range of measurements for J-13 fluids. Gas phase composition was assumed to be buffered to atmospheric values because of ready gas flow through the mountain. Bulk fluid compositions different from the "ambient" condition, variable gas-phase composition, colloid abundances, and changes to mineral distribution within and around the drifts have not been incorporated explicitly. [However, because of the conservative (far-from equilibrium) spent-fuel dissolution rates and large ranges of solubility-limited concentrations used in past TSPA calculations, the impacts of some of these potential variations may have been implicitly included.] Explicit inclusion of such information is facilitated by geochemical process models, utilizing code packages such as EQ3/6, OS3D/GIMRT, and AREST-CT, which will be used to generate compositional response surfaces for inclusion in the TSPA-VA RIP model.

The distributions of concentration limits used in TSPA-1995 are based primarily on an elicitation of chemical/geochemical experts held at Sandia National Laboratories on April 13, 1993 (Elicitation—Gauthier, 1993). Judgement of the expert panel was based on both empirical studies and modeling results, but did not include consideration of distributions used in the 1991 TSPA (Barnard et al., 1992). The results of the expert elicitation were reviewed in 1993 by the Solubility Working Group (the SolWoG is composed primarily of project scientists conducting actinide solubility/speciation studies), which recommended only two modifications to the distributions of Np and Pu. The assumptions behind the Elicitation's development of the distributions are: (1) the unsaturated zone water composition is between the composition of J-13 well water and that of UE_25p#1; (2) the solubility-limits will be determined by the far-field ambient ground-water environment; (3) the environment is oxidizing; and (4) future climate changes may cause ground-water compositional changes. A number of additional sources were used to further constrain distributions of solubility limits for the radionuclides used in TSPA-1995. The elicited solubility constraints were utilized in previous TSPAs as stochastic distributions.

6.3.3 General Description of NFGE Processes and Corresponding Models

Although the ambient geochemical system has a large capacity to moderate bulk system geochemistry, changes to the near-field geochemical environment have the potential to affect waste-package corrosion, waste-form dissolution, radionuclide solubility limits, and transport characteristics through the engineered barriers, and perhaps even through the geosphere. The geochemical environment within the potential emplacement drifts will be defined by the complex interactions among the ambient and thermally perturbed fluxes of geosphere water and gas phases through the drift, the masses of introduced materials left in the drift post-closure, and the microbial communities which may form within this region of large compositional heterogeneities (West, 1988; Murphy, 1991; Glassley, 1993; Meike and Wittwer, 1993; Wilder, 1996). A full description of the near-field geochemistry is not currently possible, however, it would include evolution of the abundances and compositions of the aqueous phase, solid phases, gas phase, colloidal phases, and microbial communities in the potential emplacement drifts for the time period of interest.

Water entering the drift will have variable composition as a function of time as a result of the heating of the system driving processes such as boiling/condensation and reaction of both heated and condensate waters with minerals and gases in the fractures of the host rocks (Arthur and Murphy, 1989; Glassley, 1993; Murphy, 1993; Wilder, 1996; Lichtner and Seth, 1996; Glassley, 1997). These reacted, or thermally perturbed, fluid compositions may flow down fracture pathways and enter potential emplacement drifts where they could undergo reaction with introduced materials or be boiled again and deposit mineral precipitates containing salts (Glassley, 1993; Murphy and Pabalan, 1994; Wilder, 1996; Lichtner and Seth, 1996). The total amounts of salts deposited within the drifts will depend to some extent on the composition of ambient water within the unsaturated zone.

Ambient water compositions measured from the Yucca Mountain saturated-zone within the tuffaceous units (as represented by samples from well J-13) are predominantly dilute sodium bicarbonate fluids with high concentrations of aqueous silica (Benson et al., 1983; Ogard and Kerrisk, 1984; Kerrisk, 1987; Harrar et al., 1990). Harrar et al. (1990) evaluated water from Well J-13 for use as a reference water composition and concluded that it could be used as such for the purpose of a base case fluid. It was noted that fluids taken from flowing fractures at Rainier Mesa had compositions similar to the J-13 values (Harrar et al., 1990). Analyzed water compositions from the unsaturated zone tuffaceous rocks (Yang et al., 1988, 1990; Peters et al., 1992; Yang, 1992) indicate that they have pH values in the range of 6.3 to 7.5 and that some constituents (Ca^{2+}, K^{+}, Mg^{2+}, SO_4^{2-}, Cl^{-}, and dissolved silica) are more concentrated than found in samples from the saturated-zone tuffaceous aquifer. However, the average HCO_3^{-} content measured in 83 water samples extracted from unsaturated-zone non-welded tuff was lower than that in the saturated-zone samples (Peters et al., 1992).

In addition to thermally driven perturbations to the flux and composition of water entering a potential drift, the flux and composition of gas into the potential emplacement drifts should be affected by the heating of the system (Murphy, 1991; Glassley, 1993; Codell and Murphy, 1992; Murphy and Pabalan, 1994; Lichtner and Seth, 1996: Wilder, 1996; Glassley, 1997). One major process affecting the in-drift gas composition is the boiling of the pore water, which is expected to drive out most of the air component of the gas from the drift environment (Murphy, 1991; Pruess et al., 1990; Murphy and Pabalan, 1994; Dunlap et al., 1997). The changes in the air mass fraction of the gas will drive changes in the water chemistry and changes to the solid materials in the drifts because of, for example, the interaction of CO_2 gas with (a) water in terms of pH controls, and (b) cementitious materials in terms of calcite formation.

During construction of potential emplacement drifts, a number of substances, which are likely to remain in the system over geologic time, will be introduced into the system to create an in-drift set of solids dominated by the introduced engineered materials, rather than by the host lithology. These materials may include a wide variety of specific compounds but there are three main categories that potentially will be abundant after closure (as part of the waste package or as structural components): steels (waste package and support, some ground support), cementitious materials (concrete liner and invert), and organic substances (within concrete mix). The reaction of these materials with the water and gas fluxing through the drift will alter the composition of water that may contact both the waste packages and waste forms, and the composition of water in which radionuclides transport through the engineered barrier system. In addition, the engineered barrier system component materials will be altered by this reaction. The concretes will alter and organic constituents may provide abundant nutrients for microbes. Microbial activity may alter pH and CO_2 fugacity within the drift. The waste forms themselves also represent substantial solid masses that will affect fluid composition within the potential drifts for some period of time (M&O, 1997).

The alteration of steels will produce Fe-oxide and hydroxide solid phases within the drift and may stabilize Fe-silicates. These phase changes will alter the sorptive properties of the EBS components and affect transport of radionuclides. Both colloids generated from the waste forms and colloids generated from steel that strongly sorb radionuclides could provide additional radionuclide transport capabilities (Meike and Wittwer, 1993; Triay et al., 1995). Besides waste-form and introduced colloids, natural colloids are present within the incoming fluid. The mass concentration of natural colloids of size > 200 nm in J-13 water was measured to be about 23 ng/ml (Triay et al., 1995b), which was similar to the value of 27 ng/ml measured by Ogard (1987) for natural colloids > 400 nm. In order for these concentrations of natural colloids to account for 10% of a particular mobile radionuclide, Ogard (1987) calculated that a sorption distribution coefficient of greater than 4×10^6 ml/g was necessary for that radionuclide. This value is much higher in general than the measured values for Pu sorption, and therefore, natural colloids are assumed to be negligible relative to the waste-form and introduced colloids discussed above.

Many of these processes cannot be represented currently in detailed mechanistic models of the chemistry completely coupled to the fluid flow and physical evolution of the system. However, pieces of the system are being constrained using experimental results (Lu et al., 1997) and models of the thermochemical behavior of the system (Wilder, 1996; Glassley 1997). For the TSPA-VA, explicit consideration of the near-field geochemical environment evolution constitutes a major step forward for directly including the potential chemical variations affecting source-term performance, however, this initial effort is only a relatively simplified representation of the complex interactions of this heterogeneous system.

The evolution of water which may be dripping into drifts is being assessed using both reaction mass transfer code packages such as EQ3/6 and REACT, and coupled reactive transport simulators OS3D/GIMRT (Wilder, 1996; Glassley, 1997). Fluid compositions measured from the single-heater test provide data to evaluate whether the models of fluid composition need to be refined. Assessment of the interaction of this water with concrete, steels, and the formation of salt crusts will also be done with these code packages, although limited equilibrium thermodynamic and kinetic data for some of these systems allow only treatment of idealized systems (e.g., cementitious systems). The fluid leaving the waste form (supplied by the waste form degradation/mobilization task) will be evaluated similarly for reaction with the underlying EBS materials, first WP steel, then invert/lining concrete. The AREST-CT code may also be used to evaluate coupled reactive transport through the materials within the drift, including the waste forms, once the dominant chemical species of the system can be identified to facilitate the construction of an idealized chemical system for input. These analyses will use the base-case gas composition for setting gas fugacities in the calculations and will be supplemented with sensitivity analyses incorporating the perturbations developed in the models addressing gas composition evolution and microbial communities effects. The colloid transport sensitivity studies will be assessed against non-colloid transport of radionuclides to the water table (see UZ transport, Section 6.8).

The assumption that the in-drift gas composition will be set by the gas flux into the drift (supplied by the thermohydrology task) is being evaluated initially using mass balance considerations for reaction of oxygen and carbon dioxide gas components with sources and sinks within the drift. If mass balance constraints indicate that there could be substantial time periods where the gas composition is affected by the source/sink terms, then more explicit calculations will be performed using reaction rates for each sink/source term built into the gas-flow codes. For the effects of microbial communities it is not possible to obtain the information about all the relevant microbial processes at the resolution that is required to interface directly with an abiotic geochemical tool like the EQ3/6 code package. We therefore have chosen to use a more simplistic approach, similar to that of McKinley et al., (1997). This approach uses abiotic processes to determine the rate at which nutrients become available to micro-organisms, and then assumes that the micro-organisms convert those nutrients to the products instantaneously, using limiting guidelines of energy availability and the availability of all the required nutrients in the proper ratio. This conceptual model is being converted into a program to do the calculations using the logic flow presented in the EMMA model (Capon and Grogan, 1991) of nutrient (C, N, P, S) and energy-limited development of microbiological activity. If the compositional perturbations from the biological activity appear substantial compared to the abiotic system, these perturbations will be incorporated into the abiotic models.

6.3.4 Issues Associated with Process Model

The key issues associated with the near-field geochemical environment were compiled into four major categories for the purposes of discussion at the three-day abstraction/testing workshop held on March 5-7, 1997: solid phases throughout the drift, the in-drift gas phase, the aqueous-phase composition throughout the drift, and colloids throughout the drift. For each of these categories, the major issues identified prior to and during the workshop are listed in tabular form below, along with the relative ranking of importance assigned to them by the experts participating in the workshop. Subsequent discussion of the issues provided four areas for development of work needed to clarify the evolution of the near-field geochemical environment: (1) the reaction of water with introduced solids, (2) the extent of microbial communities development, (3) the transport of colloidal radionuclides, and (4) evolution of the gas phase composition. An abstraction analyses plan was then developed at the workshop (and refined thereafter) for each of these four major areas, and these will form the basis for representing the near-field geochemical environment in the TSPA-VA model. These four abstraction approaches are discussed in detail in the next section. Tables 6.3-1 to 6.3-4 list the NFGE issues discussed at the workshop. More detail on these issues and their representation in the abstractions may be found in the NFGE workshop report (M&O, 1997).

The overall importance ranking (see M&O, 1997) for the issues in Tables 6.3-1 to 6.3-4 were based on four criteria. These criteria were developed so that the issues could be ranked against their potential impacts on long-term performance. The primary way the near-field geochemical environment may impact long-term performance is through changes to the engineered barrier systems that are containing the radionuclides in the near-field, resulting in a change in the source term (radionuclides and/or bulk chemistry) being supplied to the geosphere transport. The engineered barrier components include the waste form, waste package, and other engineered materials through which the mobile radionuclides may transport. Chemical changes to the in-drift environment may affect these systems via changes to the amounts and types of mobile radionuclides and the properties of the solids through which they transport to the edge of the geosphere. Therefore the four criteria chosen for ranking the issues were the dissolved radionuclide concentration, colloidal radionuclide abundances, in-drift sorption capacities, and the in-drift porosity and permeability.

The abstraction approaches discussed in the next section address all of the issues listed in Tables 6.3-1 to 6.3-4 except for nine of them. However, all of these nine issues not directly addressed are being investigated under analysis plans associated with the thermohydrology, waste package degradation, and waste form degradation/mobilization workshops, or as deliverables under existing work scopes. More detail is given in the NFGE workshop report (M&O, 1997).

6.3.5 Major Assumptions and TSPA-VA Abstraction Approach

The issues listed in Section 6.3.4 have been combined into four abstraction plans: (1) a water-solids chemistry model; (2) a colloid-facilitated radionuclide transport model; (3) a model dealing with the influence of microbial environments; and (4) a model for gas-composition evolution. The primary model affecting the TSPA representation of the EBS is the water-solids model, which supplies the fluid compositions through time that react with the waste packages, the waste forms, and the underlying EBS components, and the composition of water entering the geosphere for transport. Results from the models of microbial communities and the gas-phase composition evolution will be fed mainly back through the water-solids chemistry model. (Although parameters such as the oxygen fugacity through time may be used by waste package and waste form models directly). The colloid sensitivity studies will be used to compare releases of Pu transported as purely aqueous species to situations including colloidal Pu. Results of the water-solids chemistry model for use in the total system performance assessment model will be abstracted EBS solids' evolution scenarios and fluid composition response surfaces for various regions of the EBS. The approach for using these abstractions within the RIP TSPA model is to include the output from the water-solids chemistry model as response surfaces (multidimensional tables) that set the chemical environment within the RIP EBS "cells". These RIP cells are basically equilibrium batch reactors that have advective and diffusive components of transport into and out of the cell.

Key processes occurring within the cells (besides transport into and out of a cell) are degradation of materials and redistribution of radionuclides amongst the various phases. These physical-chemical processes are affected by some of the key NFGE output parameters, such as pH and carbonate concentration. By coupling a time history of these NFGE compositional parameters to each cell environment, the NFGE model is effectively coupled to the waste-form degradation model, waste-form mobilization model (transport of radionuclides through perforations in the waste package), and EBS transport model. Thus the basic modeling approach is to provide response surfaces from the NFGE model to the various RIP cells, which represent a series linkage of discrete spatial domains containing different materials. A schematic of this type of approach is shown in Figure 6.3-1, which is a response surface of pH at a given time at discrete locations within the drift.

Water-Solid Chemistry Model. The primary outputs of this model are the water compositions that (a) are likely to react with the waste package and the waste form and (b) form the medium for transport through the engineered barrier system. The primary products of this effort are expected to be time-dependent bounds on the ranges of dissolved constituents that are needed as inputs to subsystem models like waste package corrosion, waste-form degradation, and solubility-limited radionuclide concentrations (e.g., pH, Cl^-, F^-, SiO_2°, CO_3^{2-}, Ca^{2+}, Na^+, and SO_4^{2-}).

Analyses will be conducted over a number of scenarios including (1) variable starting water and gas compositions and extent of equilibration for reaction with concrete and steel in the base cases, and (2) crushed-tuff backfill in the sensitivity cases. Specific scenarios representing the stages of the pathway for the water flow prior to contacting the waste form will be constructed. These will represent the potential for fluids to have reacted with evolved cementitious materials and evolved steel prior to contacting the waste. In addition, scenarios will be constructed for idealized compositional pathways followed by the water leaving the waste package.

The extent of evolution of cementitious materials will be represented by various mineral assemblage scenarios for the degraded cement. These scenarios will be tied to the system evolution through temperature dependent switches for the various mineral phase transitions, which will be applied to the thermohydrologic results. Incoming fluids will be reacted with these cementitious material representations via geochemical reaction path codes (e.g., EQ3/6) to estimate the steady-state fluid composition that will be taken as the fluid leaving the material. This resultant fluid will then be reacted similarly with the next material in the sequence. Resulting fluid compositions at different points within the drift will then be tied to the evolution of the in-drift materials to develop the scenarios of fluid composition spatial and temporal evolution. Given adequate time, coupled models of fluid flow and chemical reaction (such as OS3D/GIMRT and AREST-CT) will be applied to more explicitly evaluate the simultaneous evolution of solids and water. If the gas evolution and microbial communities models indicate that large perturbations from the assumed base-case gas compositions are expected, these will be directly incorporated into the water-solid chemistry calculations.

Colloid-Facilitated Radionuclide Transport. The main objective of this abstraction is to conduct sensitivity studies to assess the contribution to radionuclide release from colloids and, if shown to be substantial compared to dissolved and gaseous radionuclide releases, provide an abstracted model for TSPA-VA. A simplified model will be developed to examine the effect on Pu release from intrinsic Pu colloids (Pu hydrous oxide polymers) and Pu sorbed on nonradioactive colloids (specifically iron oxides). These analyses will consider interaction of Pu with the solids in the drift and the rock minerals in both the rock matrix and fracture system.

To simulate sorption on pseudocolloids, forward and reverse rate constants will be used. These parameters will be estimated, considering the available sorption sites on colloids, or constrained by experimental determinations being made on the project. The concentration of nonradioactive colloids will be based on stability arguments and limited measurements for the formation/stability of Fe-oxy-hydroxy colloids. In addition, concentrations of Pu intrinsic colloids, and sorption information for interaction of Pu with the host rock will also be provided.

Stability information is available for some colloids, including iron oxides, clays, and silica. This sensitivity analysis will be performed using only iron oxide(hydroxide) as the nonradioactive colloid. From the information sources listed above, the source term for Pu concentrations as intrinsic colloids will be developed, as well as an estimate of Pu associated with iron oxides/hydroxides in the engineered barrier system, as functions of pH and solution ionic strength.

Two flow/transport models will be tested: a one-dimensional, Weeps-like (Wilson et al., 1994, M&O, 1996) calculation in which fracture transport of colloids is unaffected by matrix interactions; and, if there is sufficient time, a detailed, two-dimensional transport calculation using FEHM (LANL, 1997). The detailed flow and transport models will use hydrologic parameters developed in the EBS transport activity of the waste-form degradation/mobilization effort. Special conditions for colloid transport, such as restricting colloid transport to fractures, will be developed and included in the transport model. Pu will be tracked in four forms: Pu in solution (in the groundwater); Pu sorbed onto host rock minerals (matrix and fracture); intrinsic Pu colloids (e.g., Pu hydrous oxide polymers); Pu pseudo colloids formed by the interaction of dissolved Pu (aq) with nonradioactive colloids and colloidal Pu (intrinsic colloid) with nonradioactive colloids.

The near-field geochemical environment aspects of the colloid sensitivity study are being directly incorporated into the unsaturated zone transport sensitivity study. The comparative measures (colloidal Pu transport vs. purely aqueous Pu transport) will be made at the water table as part of the UZ transport effort. If colloidal transport is deemed to be important, based upon the above sensitivity studies, then some form of colloidal transport model will be combined with the FEHM particle tracker that is to be used to simulate radionuclide transport in two or three dimensions in the unsaturated zone (see Section 6.8).

Effects of Microbial Communities. The main objective of this model is to develop response surfaces or analytic approximations that bound the development of microbial communities and their corresponding effects on solution pH and gas composition evolution (mainly CO_2) after emplacement. This work will be accomplished by producing a model that evaluates the microbial community activity and its effects on the chemical environment based on the nutrient supply to those microbes and the conditions under which they exist.

The products of this model are (1) a spatial-temporal description of microbially-dominated pH, (2) the temporal description of microbially generated CO_2, and (3) the temporal evolution of microbial population (i.e., biomass) as affected by nutrient availability, relative humidity, temperature, microbial reaction rates, and initial microbial community. These outputs will be cast in the form of response surfaces for these above parameters and fed to the Water-Solid Chemistry model and the Gas Composition Evolution model where they will be incorporated as extended sensitivity analyses and assessed against the abiotic results to gauge the magnitude of the microbial input to the geochemical interactions of the system.

The model developed will be based on previous models for nutrient-driven microbial activity and will incorporate features specific to the near-field geochemical environment of this system, such as the unsaturated state of the system, and the possibility of aerobic as well as anaerobic activity. Definition of the domain under which microbes can be active will be input into the model including variable saturation limits, temperature limits, and radiation limits on microbial activity.

Gas Composition Evolution in the Drift. This model will address potential temporal changes in four gas constituents (H_2O, CO_2, O_2, and N_2), where the H_2O component is given by the thermohydrologic models, and the nitrogen will only represent the remainder of the "air". The main objective is to assess the competition between external drives (i.e., the gas flux into the drifts) and in-drift source/sink terms (e.g., alloys, concrete) for these gas constituents. The results would be given as response surfaces (with uncertainties) for the O_2 and CO_2 content of the gas in the drift through time. These results would be fed to both the water-solids chemistry model for incorporation, as well as to the waste package degradation and spent fuel dissolution models for direct constraints on the abundance of oxygen in the drifts.

Initially, simple mass balance calculations between incoming gas and the capacity of source/sink terms to affect that incoming composition will be performed to assess the need for doing more complex interaction calculations. The analyses will be done for a range of possible system permeabilities and for two locations within the repository (center and edge) to evaluate sensitivities in the system. The thermohydrologically driven gas flux will be compared to the masses of sources/sinks of gas within the drift associated with the introduced materials, as identified by the Repository Design and Waste Package Design Organizations. The response surfaces will constitute direct inputs to the waste package and waste form subsystems, and would be utilized by other abstraction models developed for the NFGE.

Constraints on the gas flux will be used for a range of permeabilities (3 values), and from two areas of the potential repository (middle and edge). The masses of cementitious materials and metals and alloys will be used to constrain many of the source/sink terms used in the calculations. For example, we will analyze integrated air mass flux across the repository as a function of time to derive the time needed to supply enough oxygen to oxidize all the carbon steel. This will provide a simple constraint on the length of time oxygen could be completely removed (effectively) from the drift atmosphere. This time can then be compared to performance time-scales and the benefit assessed in terms of enhanced performance of the inner barrier or waste form in a low oxygen environment.

If this first set of calculations indicates that the system gas composition is not controlled by inflow of air, then we will perform more detailed calculation of flow including reaction rates of dominant sources and sinks for the constituents of interest and evaluate the effect of compositional gradients on the gas-transport rates.

Conceptualized evolutionary paths of gas composition from the process-level information will be used to generate response surfaces as function of time. These surfaces will represent the average values but will have some estimate of the uncertainties in those values.

6.3.6 Base Case and Sensitivity Cases

The near-field geochemical environment model results will be used by other EBS subsystem models, such as waste package degradation and waste form degradation/mobilization. The base case EBS models will be implemented in TSPA-VA using the RIP compartment model. As defined in Section 6.3.3, the models will discretize the EBS into several components. This will allow geochemical differences between components to be readily incorporated, as well as appropriately facilitate the model of transport from the waste form through the rubblized waste package (corrosion products) and invert/liner materials. Figure 6.3-2 shows this compartmentalization and the schematic influence of the NFGE on each RIP cell. Within the RIP cells, the near-field geochemical environment base-case results will be used to set the compositional variables for water and gas composition, and solid phases as a function of time, as described below.

The base case near-field geochemical model consists of (1) a set of idealized initial materials within the model emplacement drift defined from the introduced materials information provided by the Repository Design Group; (2) time-dependent water and gas fluxes into the drift and in-drift temperatures provided by the results of the thermohydrologic base case calculations; (3) time-dependent compositions of incoming thermally perturbed water and gas compositions based on the analyses/interpretations/models of William Glassley (LLNL) for the single-heater test results; (4) idealized scenarios for the time evolution of the major solids in the drift (i.e., concrete and steel) based on the experimental work/models of Annemarie Meike (LLNL), which will be presented as a series of stages having discrete mineralogies; (5) time-dependent composition of the water leaving the waste forms supplied by the waste-form degradation/mobilization tasks; (6) a set of disequilibrium reaction mass transfer calculations that simulate the reaction of water from #3 above with the scenarios from #4 for each stage—these will be performed on a single material until equilibrium/steady state is achieved, and the resultant fluid composition will be used for reaction with the next material (e.g., incoming water reacts with concrete mineral scenario A and resultant water composition is reacted with steel mineral scenario A, etc); and (7) a set of disequilibrium reaction mass transfer calculations that simulate the reaction of water from #5 above with the scenarios from #4 for each stage—these will be performed on a single material until equilibrium/steady state is reached, and the resultant fluid composition will be used for reaction with the next material (here the reaction sequence is steel mineral scenario A *then* concrete mineral scenario A). Figure 6.3-3 is a schematic representation of the locations of response surfaces for fluid compositions to be provided by the NFGE model. For locations 1, 2, and 3 in this figure, the fluid compositions will be utilized by process models external to RIP, whereas fluid compositions at points 4, 5, and 6 will be fed directly into RIP cells as response surfaces.

The idealized introduced materials for the base-case (see Figure 6.3-3) are comprised of concrete and steel and the masses and compositions are defined from the information provided by the Repository Design and Waste Package Design Groups concerning compositions/abundances/distributions of introduced materials that will be left in potential emplacement drifts post-closure. The concrete liner and invert will be represented as will the steel of waste packages, pedestals, and rails, although their compositions may be somewhat idealized. For example, the organic materials in the concrete mix design as described in the Design Report on materials for emplacement ground support (M&O, 1997b) will not be included explicitly, but will be used in sensitivity analyses bounding development of microbial communities.

Sensitivity analyses will be performed in a number of areas. First, the evolution of gas composition (the oxygen and carbon dioxide components) via reaction with materials in the drift will be evaluated using mass balance assessments of the major sources and sinks for these constituents relative to their supply in the gas fluxing into the drift. Should there be indication of substantial times where these gas species would be controlled more by the source/sink terms than the gas flux, then these reactions and their effects on water composition will be explicitly incorporated into the water-solid chemistry model. Bounding assessments on microbial communities developments will similarly provide potential changes to both gas and fluid compositions. If these appear substantial relative to the abiotic chemistry then they too will be directly incorporated into the water-solid chemistry model. The sensitivity analyses for colloids will be handled primarily in the unsaturated-zone transport activities (Section 6.8). In addition to the above sensitivity studies, further possible fluid pathway scenarios "upstream" of the waste package will be investigated. This includes allowing water to "miss" reaction with concrete, reaction with salt precipitates formed during the boiling period, and potentially reaction with backfill/drip shield materials. For various thermohydrologic scenarios the mineralogic scenarios will have adjusted time intervals which will change the length of time a particular fluid composition is extant. For the gas composition evolution, evaluation of a range of permeabilities will be done to check how much gas flux varies. Finally, more coupled calculations involving the fluid flow coupled explicitly with solids and gas reactions will be performed if the models can be constructed within the time-frame of the TSPA-VA.

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Table 6.3-1. Issues Associated with Solid Phases Throughout the Drift

Issue #	Issue Name
1.11	Volume and flux of water in drift
1.1	Compositions, abundances, and distribution (cement, alloys, organics, microbes, ceramics)
1.5	Aqueous and gas reactions on materials
1.6	Aqueous and gas reactions (corrosion) on WP
1.9	In-drift system open or closed
1.8	Temporal heterogeneity
1.1	Microbial processes
1.2	Thermal Effects on materials (excluding WP)
1.3	Mineral precipitates (salts)
1.4	Thermal effects on WP
1.7	Spatial (in-drift) heterogeneity

Table 6.3-2. Issues Associated with the In-Drift Gas Phase

Issue #	Issue Name
2.9	Gas flux
2.3	Reactions with solids & microbes (excluding waste package)
2.4	Reactions with waste package
2.6	Thermal effects (water reactions)
2.8	Temporal heterogeneity
2.2	Climate effects
2.5	Reactions with waste forms (radiolysis)
2.1	Ambient pore gas
2.7	In-drift spatial heterogeneity

Table 6.3-3. Issues Associated with the Aqueous Phase Composition Throughout the Drift

Issue #	Issue Name
3.3	Aqueous phase reactions with major introduced materials (excluding WP)
3.1	Open vs closed system
3.4	Aqueous phase reactions with WP
3.9	Temporal evolution of aqueous phase composition
3.2	Perturbed water composition entering drift
3.5	Aqueous reactions with waste form
3.6	Thermal effects on aqueous phase compositions
3.7	Aqueous phase reactions with evaporite minerals
3.11	Microbial process effects on aqueous composition
3.1	Ambient water composition
3.8	Spatial variability of aqueous fluid compositions

Table 6.3-4. Issues Associated with Colloids Throughout the Drift

Issue #	Issue Name
4.9	Reversibility of radionuclide sorption onto colloids
4.5	Water-composition effects
4.3	Waste form
4.2	Other (introduced materials in rock)
4.7	Temporal heterogeneity
4.8	Microbial processes
4.4	Temperature effects
4.1	Natural colloids
4.6	In-drift spatial heterogeneity

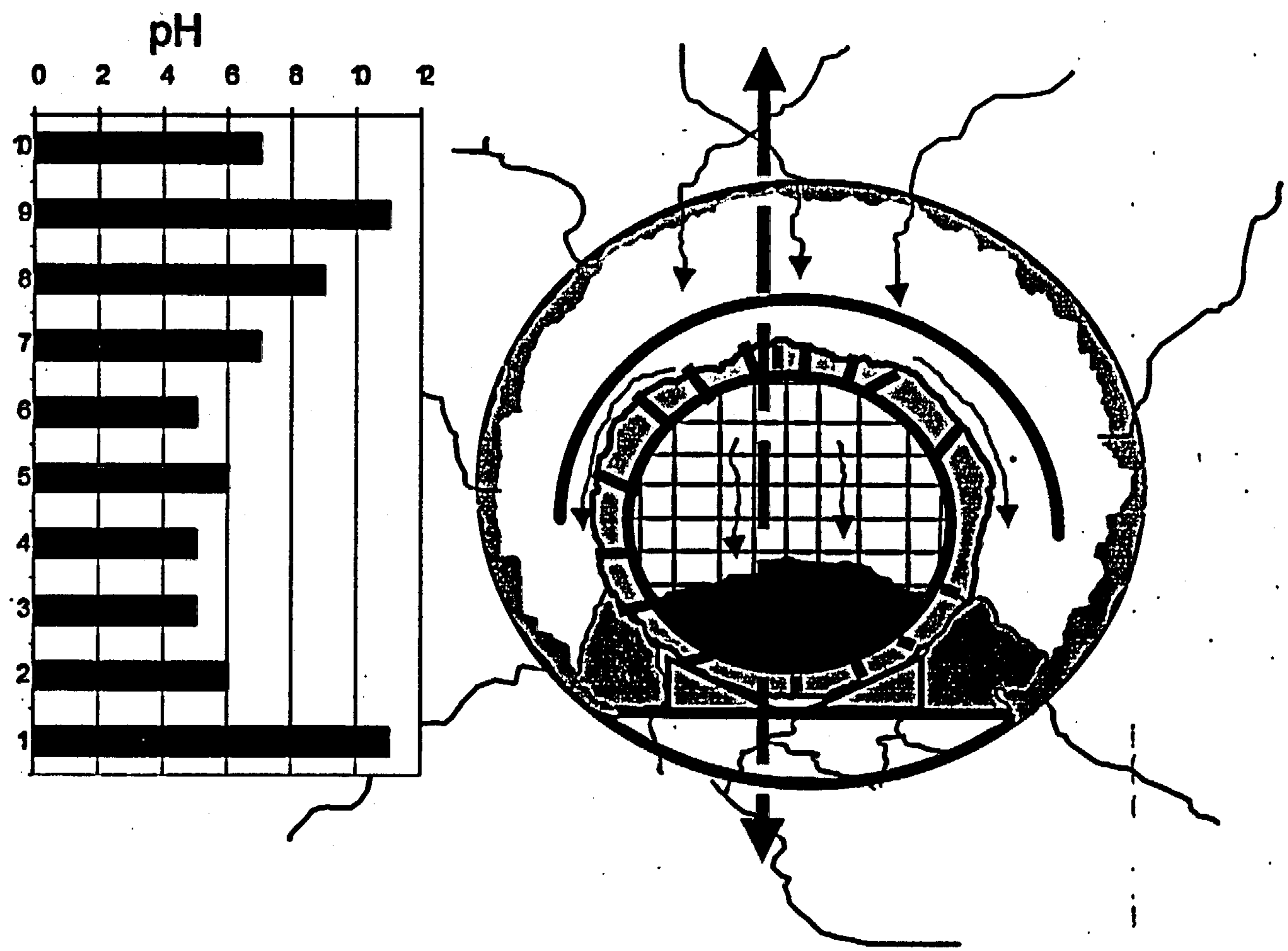

Figure 6.3-1. Example response surface for pH as a function of discrete location within the EBS, at a given time. pH generated by the NFGE model.

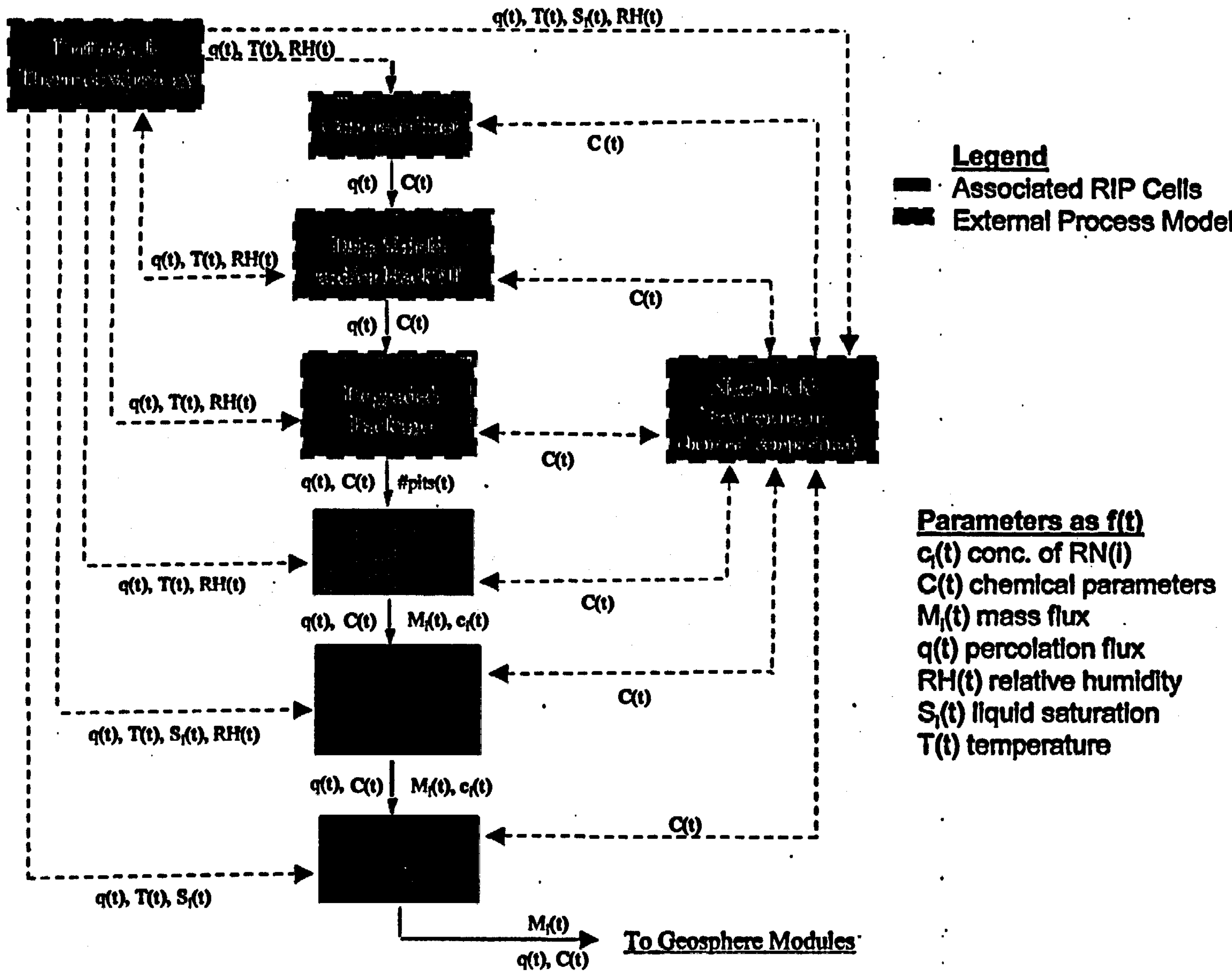

Figure 6.3-2. Coupling of near-field environment model with other EBS component models.

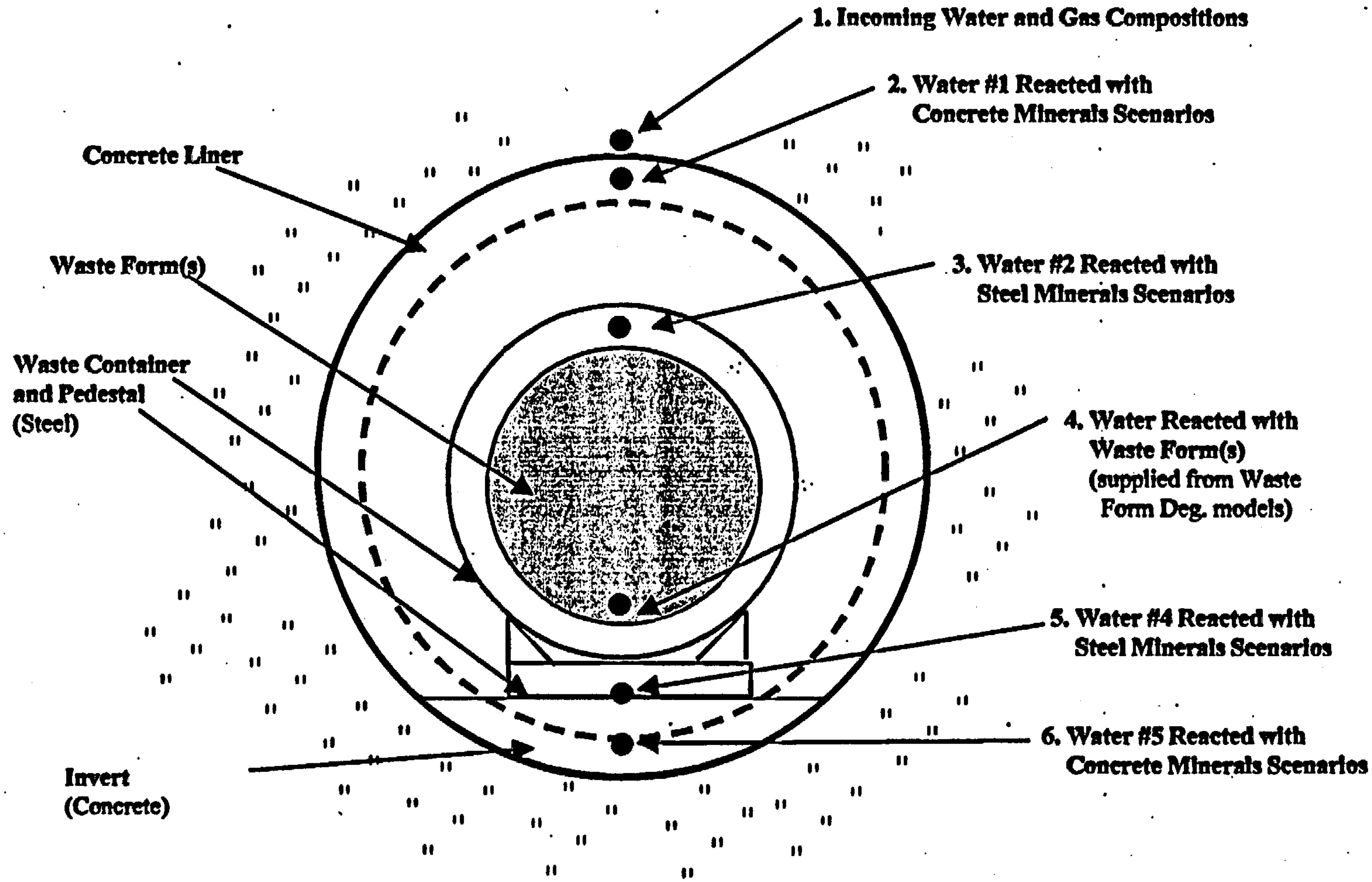

Figure 6.3-3. Schematic representation of in-drift materials included in, and locations of water compositions calculated for, the near-field geochemical environment base-case for TSPA-VA.

6.4 WASTE PACKAGE DEGRADATION

Joon Lee, Jerry McNeish, S. David Sevougian

6.4.1 Introduction

General. The important components of the EBS base case at some time after emplacement are shown in Figure 6.4-1. This figure indicates the numerous engineered components which potentially affect the degradation of the emplaced waste packages. Alteration of the incoming fluid rate and chemistry will affect the degradation of the waste packages. Other significant contributors to the degradation of the waste package are the temperature and relative humidity in the drift and the water contact mode. The waste package design was described in Section 4.1.1. It consists of an outer corrosion allowance material (10 cm thick) and an inner corrosion resistant material (2 cm thick).

The primary role of the waste package degradation model is to provide information on the lifetime and overall degradation of the waste package. The degradation description is to be developed as a function of the environment of the waste package. This model is very significant in the overall TSPA because it significantly contributes to determining the rate and time of release of radionuclides from the waste package.

A drip shield (with associated backfill) has been recently proposed as a design option to divert dripping water and thus to prevent direct contact of any dripping water with the waste package (Bailey, 1997). The drip shield configuration will <u>not</u> be considered part of the base case for TSPA-VA, but will be evaluated in the sensitivity cases. The degradation mechanisms and rates for the drip shield are highly uncertain. Another uncertainty associated with the drip shield performance is the alteration of thermo-hydrologic processes in the near-field causing condensation of moisture underneath the drip shield leading to dripping on the waste packages. The performance effect of these uncertainties depends on the design, materials and degradation of the drip shield. But the component holds promise from a performance perspective if it is able to reduce the amount of percolation flux which reaches the waste packages.

Input. The key inputs for evaluating the waste package degradation are shown in Figure 6.4-2. These inputs include:

- Thermo-hydrologic conditions in the drift (i.e., temperature, relative humidity, liquid saturation and in-drift dripping flux) as a function of time and location. The thermo-hydrologic modeling will provide the temperature, RH, and liquid saturation. A further abstraction will produce the dripping flux rates and locations.

In TSPA-1995, the waste package degradation model is the most detailed such code to date. The model included components for outer barrier humid air and aqueous corrosion, inner barrier pitting corrosion, and galvanic protection (Lee, et al., 1996a; Atkins, et al., 1996). The model also included evaluation of variability in corrosion among waste packages as well as uncertainty in the critical RH for initiation of humid-air and aqueous corrosion. The outer barrier corrosion models (both humid-air and aqueous) were developed using data from the literature (Lee, et al., 1996b). Essentially, the corrosion rates were determined by developing an empirical model from data available on corrosion of mild steel. The inner barrier pitting model was based on an expert elicitation (Andrews, et al., 1994). The galvanic protection module was based on expert judgement (McCright, 1995) and provided for a delay in the pitting corrosion of the inner barrier until a certain percentage (user defined) of the outer barrier had corroded. The galvanic protection model is expected to be significantly revised for TSPA-VA.

Effects of variability in exposure conditions including rockfall and backfill on waste package degradation were not explicitly considered in previous waste package PA modeling. One approach developed and implemented in TSPA-1995 was to utilize the uncertainties in individual corrosion models (i.e., humid-air general and localized corrosion models and aqueous general and localized corrosion models for the carbon steel outer barrier) as the waste package model variability. Half of the uncertainty in the models was assigned to represent the effects of variability in exposure conditions across the repository (referred to as waste-package to waste-package variability), and the remaining half of the model uncertainty was used to represent variable corrosion rates within a single waste package (referred to as pit to pit variability). That approach used in TSPA-1995 was not based on data or field observations.

Other potentially important corrosion modes such as stress corrosion cracking (SCC) and microbiologically influenced corrosion (MIC) have not been included in previous TSPA waste package models. In addition, a number of additional processes which contribute to waste package degradation have not yet been incorporated in the waste package degradation model. These processes include rockfall damage, potentially preferential attack on weld zones, salt deposits from dripping water, and water chemistry effects on waste package degradation.

6.4.3 General Description of Process Model

The current subsystem model for evaluating degradation of the waste package is WAste Package DEGradation (WAPDEG) model (M&O, 1996). The WAPDEG model currently evaluates the degradation of the waste package outer barrier based on an empirical formulation developed from experimental data and the nickel-based inner barrier based on the model developed from an expert elicitation. Individual corrosion models for the carbon steel outer barrier and the nickel-based inner barrier, which are based more on the mechanistics of corrosion processes are under development and/or improvement. First-cut models of MIC for the barriers are being developed. These models, once completed or updated, will be incorporated into the WAPDEG model. ..

For modeling the outer barrier corrosion, both humid air and aqueous corrosion as a function of exposure time, temperature and relative humidity (only for humid-air corrosion) are simulated in the model. Localized variations of the outer barrier corrosion are represented by a pitting factor as a multiplier to the uniform general corrosion depth. The model also includes the spalling of corrosion products from the outer barrier (Lee, et al., 1997). The primary inputs to the model are temperature and relative humidity at the waste package surface as a function of time, waste package design (such as the CAM and CRM barrier thickness), and pitting factor for localized corrosion of the outer barrier. The updated outer barrier model is intended to include dependencies on the water chemistry, salt scale formation, and dripping water.

The current model assumes the inner barrier subject to aqueous pitting corrosion only and calculates distribution of pitting rates as a function of temperature. Also, a simple galvanic protection model has been used which only allows pitting corrosion of the inner barrier after a certain percentage of the outer barrier thickness has been corroded. This galvanic protection model will be significantly revised for TSPA-VA and will not be included in the base case. The updated WAPDEG model is expected to include pitting corrosion, active crevice corrosion, and the interaction between inner and outer barrier including: 1) crevice formation between the outer barriers, and the outer barrier corrosion product precipitates and the inner barrier; 2) pH suppression in the crevice due to the hydrolysis of dissolved metal ions from corrosion of both the barriers, and 3) galvanic coupling between the barriers, and 4) the accumulation of corrosion products inside the crevice. The inputs to the inner barrier model include the waste package surface temperature to determine the penetration rate, or pit growth increment. The updated inner barrier model will include a better defined threshold for pitting corrosion initiation based on local crevice solution chemistry, a revised temperature dependence of pitting rate and time-dependent pit growth. The updated model will include a general corrosion model of the inner barrier. The outputs from the combined outer barrier and inner barrier corrosion model include the time-history of first pit penetration for the waste packages and the time-history of subsequent pit perforations for the waste packages.

The MIC has not been explicitly included in the previous TSPA waste package degradation analyses, though one could argue that it was embedded in the corrosion data from natural exposure conditions, which were used to develop corrosion models for the carbon steel outer barrier in WAPDEG. In TSPA-VA, the MIC is expected to be modeled as localized corrosion incorporating additional constraints due to temperature, water availability, nutrient availability, and pH.

The recently proposed drip shield was not considered mechanistically in previous TSPA analyses. Simple evaluations which assumed the properties and lifetime of the drip shield (i.e., no dripping on the waste package) have been conducted. No additional work has been conducted to develop a process level model to evaluate the long-term degradation of a drip shield. Due to the lack of degradation information, expert judgement will be relied on to define scenarios for the evaluation of the system which includes the drip shield. These analyses will not be included in the base case.

6.4.4 Issues Associated with Process Model

The waste package degradation issues determined at the Waste Package Degradation Workshop to be most important to performance are listed by importance in Table 6.4-1 for the four major areas: 1) carbon-steel outer barrier corrosion, 2) nickel-based inner barrier corrosion, 3) microbiologically influenced corrosion, and 4) uncertainty including rockfall, premature failure, and structural failure (M&O, 1997a). It is important to note that the workshop focussed more on model development and less on abstraction for TSPA-VA.

Carbon Steel Outer Barrier Corrosion. The carbon-steel outer barrier corrosion plan is to develop a model or models which meet the following objectives;

- Develop a model of humid-air general corrosion for the carbon-steel outer barrier for use in waste-package degradation model for TSPA-VA.
- Develop a model of aqueous general corrosion for the outer barrier for use in waste-package degradation model for TSPA-VA.
- Develop a model to represent localized corrosion (or variation in general corrosion depth) of the outer barrier in humid-air and aqueous corrosion conditions
- Exercise the models to investigate sensitivity of waste package degradation to the carbon-steel outer barrier corrosion

The key hypotheses for this plan are as follows:

- Humid air corrosion can be represented as a function of relative humidity, temperature, salt scale formation, and water dripping.
- Aqueous corrosion can be represented as a function of pH, temperature and water chemistry, relative humidity, and water contact duration.
- Localized variations in corrosion on a single package can be represented by a "pitting factor" as a multiplier on the (average) general corrosion depth. The multiplier may vary as a function of corrosion depth.

The primary results of the modeling which are provided as inputs to Waste Package PA and TSPA-VA are listed below:

- Abstracted model for "critical" relative humidity for initiation, and propagation of humid-air corrosion as a function of relative humidity, temperature, and salt deposit rate.
- Update/modification of the TSPA-1995 humid-air corrosion model to include better representation of temperature, relative humidity, and salt-deposit effects.
- Abstracted model for "critical" relative humidity for transition from humid-air corrosion to aqueous corrosion as a function of relative humidity, temperature, and type of salt.
- Update/modification of the TSPA-1995 aqueous corrosion model to include better representation of temperature, and water chemistry effects.
- Model for localized corrosion (or variations) of outer barrier in humid-air and aqueous conditions.

Corrosion Resistant Inner Barrier Corrosion. The corrosion-resistant inner barrier corrosion model plan objectives are presented below:

- Develop an inner barrier corrosion model to predict the rate of penetration of the inner barrier, which is comprised of corrosion resistant material (CRM), as a function of the near field environment (NFE) (temperature; humidity; in-drift water dripping; and the chemistry of the contacting water).
- Assume penetration of the CRM is due to localized corrosion: pitting and active crevice corrosion.
- Account for the interaction between the outer and the inner barrier including such interactions as pH suppression in the crevice due to the hydrolysis of dissolved metal ions from corrosion of both barriers; crevice formation between the corrosion product precipitates and the CRM; galvanic coupling between the barriers; and the accumulation of corrosion products. Several of these effects will be accounted for with a NFE correction (calculation of pH and mixed potential) applied at the interface between the inner and outer barriers.
- Account for microbial action, such as the conversion of Fe(II) to Fe(III), in this interfacial NFE correction.

The key hypotheses for the inner barrier corrosion model are:

- The inner barrier will be exposed in patches as the outer barrier degrades. Each exposed area (or "patch") can be subdivided into three generic zones (M&O, 1997a). These zones are defined as: Zone 1, the CRM will be directly exposed to the NFE, via humid air or a thin layer of oxygenated and acidified water; Zone 2, the CRM will be exposed to a thin layer of acidified water, with a gradient in oxygen concentration; and Zone 3, the CRM will be exposed to a thin layer of acidified and deoxygenated water.

- Penetration of the outer barrier will be by either (a) humid air corrosion or (b) aqueous corrosion.

The key inputs to waste package PA and TSPA-VA are as follows:

- General corrosion rates of the outer and inner barrier (CAM and CRM) surfaces in the crevice, as well as the accumulation of precipitated corrosion products in the crevice areas.
- Predictions of pit nucleation and growth on the CRM surfaces that lie in the three zones. Statistical distributions of pit density and depth, as well as the cumulative perforated-area of waste container will be calculated as functions of time, temperature, episodicity and flow of water onto the package, and chemistry of flow onto package.
- The fraction of failed containers will be calculated as a function of time, temperature, episodicity and flow of water onto the package, and chemistry of flow onto package.

Microbiologically Influenced Corrosion (MIC). The model for microbiologically influenced corrosion (MIC) has the following objectives:

- Develop the best model(s) possible in the time available for TSPA-VA,
- Identify sources of information that can be acquired to test the model(s) (i.e., literature, laboratory testing, natural analogues), and
- Exercise the model(s) and present the results to a body of experts.

The key hypothesis of this model is that MIC can be modeled as localized corrosion incorporating additional constraints such as: temperature, water availability, nutrient availability, and pH.

The primary inputs to Waste Package PA and TSPA-VA are as follows:

- First cut model(s) with descriptive material,
- Available parameter value (or range of values) used in the model(s), and
- Preliminary results.

The models are intended to be incorporated into the waste-package degradation model.

Effects of Variability in Near-Field Conditions, Manufacturing and Materials on Waste Package Degradation. The final plan from the workshop was to evaluate the effects of variability in near-field conditions, manufacturing and materials on waste package degradation

- Develop models/abstractions to represent variability in waste-package materials, waste-package manufacturing, and near-field conditions including rockfall
- Develop methods to incorporate the models/abstractions for the variabilities into waste-package degradation model
- Exercise the models/abstractions to investigate the sensitivity of waste-package degradation to the variabilities

The key hypotheses for this work are as follows:

- Effects of variability in waste-package materials, waste-package manufacturing, and near-field conditions including rockfall can be represented by sampling over individual model parameters.
- There is a physical basis for a localization factor to represent enhanced corrosion at the welded regions of the carbon-steel outer container
- Enhanced corrosion at the welded regions of the corrosion-resistant inner container can be represented by changes in the corrosion model parameters
- Effects of rockfall/backfill on the waste-container corrosion processes can be represented as providing preferential sites for localized corrosion processes. Rockfall/backfill would form crevices in contact with the waste package and provide wetter conditions at the contact points.

The primary inputs to waste package PA and TSPA-VA are listed below.

- Methods/approaches to represent variability in corrosion rates over the surface of a single waste package and among waste packages across the repository will be provided to the waste-package degradation model.
- Methods/approaches to represent enhanced corrosion due to rockfall and at the welded regions of the corrosion-resistant inner container will be developed and provided to the waste-package degradation model.
- Localization factors (or a range of the factors) to represent locally enhanced corrosion of the outer container (for the welds and rockfall/backfill) will be developed and provided to the waste-package degradation model.

6.4.5 Major Assumptions and Approach to Abstraction of Process Model for TSPA

The WAPDEG model provides a description of waste package degradation which occurs as a function of time and repository location for specific design and thermo-hydrologic modeling assumptions. This information can be presented to the TSPA model (RIP) in several different formats. The format used in TSPA-95 was both a waste package failure distribution (defined as the first pit perforation), and subsequent pitting perforation distribution defined as a function of time. In the abstraction of the WAPDEG results for RIP, waste packages were grouped into eight bins according to their failure times, and a representative pitting perforation time-history for the waste packages within each bin was developed. This approach used 8 discrete bins to represent the pitting degradation for packages failing within that bin. A proposed approach for TSPA-VA is described briefly below.

In TSPA-VA, the waste package degradation will be modeled by dividing the waste package surface into "patches" and populating the corrosion rates stochastically over the patches, depending on the local corrosion conditions. A schematic for this approach is shown in Figure 6.4-3. The "patches" approach is an attempt to explicitly represent the variability in corrosion rates within a single waste package and to address multi-corrosion modes within a single waste package at a given time. Variability in waste package degradation across the repository due to varying exposure conditions will be modeled by incorporating explicitly the spatial distribution of the exposure conditions. The exposure conditions intended to be included in the waste package degradation modeling are temperature, relative humidity, in-drift water dripping, pH and chloride concentration of the contacting water, and oxygen partial pressure. Effects of varying degrees of galvanic protection of the inner barrier on the waste package degradation will be modeled by stochastically varying galvanic protection measures. Also, variability in waste package degradation due to the uncertainty in waste package fabrication (such as welding, degrees of contact between the two barriers, and efficiency of relief of various stresses) will be modeled by stochastically representing the latest design and fabrication data. The effect of rockfall on waste package degradation will be modeled using the data from the latest thermo-mechanical analysis on the magnitude and frequency of rockfalls.

The humid-air and aqueous corrosion models for the carbon steel outer barrier (Lee, et al. 1996b), which were used in TSPA-1995, will be refined and improved by incorporating additional site-specific data from the comprehensive corrosion testing programs at LLNL (McCright, 1997). The pitting factor approach used in TSPA-1995 to represent localized variations of carbon steel corrosion will be revised significantly to represent such localized variations more realistically. Effects of salt deposits on carbon steel corrosion will be added to the existing models. Dependence of carbon steel corrosion on pH of the contacting solution and oxygen partial pressure will also be added to the existing aqueous corrosion model.

A detailed process-level corrosion model for the nickel-based inner barrier, which incorporates the mechanisms of corrosion processes and stochastic features of localized corrosion (pitting and crevice corrosion) of corrosion-resistant materials is being developed for use in TSPA-VA at LLNL (Farmer, 1997). The process-level model will be used to evaluate a wide range of exposure conditions of temperature, pH and chloride concentration in pits and crevice. The results (i.e., pitting and crevice corrosion rates) will be abstracted into a multi-dimensional lookup table or response surface as a function of the exposure conditions and time, which will be implemented into the waste package degradation model (WAPDEG).

The results from the MIC testing and modeling program underway at LLNL will be incorporated to develop abstractions for the MIC effects on waste package degradation. The information from the current MIC testing and modeling will not be mature enough to be included in the base case for TSPA-VA, but the results will be utilized for sensitivity studies for TSPA-VA. The MIC testing on carbon steel is expected to provide an enhancement factor (or multiplication factor) to the abiotic aqueous corrosion rate (i.e., at the corresponding exposure conditions of time, temperature, pH and oxygen partial pressure, but in the absence of microbe activity). The MIC testing results for the nickel-based corrosion-resistant inner barrier will provide perturbed localized chemical conditions underneath the microbe colony, which would provide crevice-like conditions and is referred to as underdeposit pitting corrosion (Brennenstuhl, et al., 1990).

Waste Package Degradation Expert Elicitation (WPDEE). Expert elicitations are underway to evaluate the important issues to long-term waste package degradation. The final report is due in mid-August (M&O, 1997b). Additional information from the WPDEE will be incorporated into the base case to the extent feasible. In particular, for the carbon steel outer barrier model, the expert elicitation will provide information on the threshold for initiation of both humid-air and aqueous corrosion, the effect of water drips on the corrosion rate, and the representation of "localized variations" of corrosion emphasizing the long-term corrosion effects.

For the corrosion-resistant inner barrier, the expert elicitation will provide information on the threshold for initiation of localized corrosion, probability of pit generation as a function of exposure conditions (temperature, pH, and chloride concentration), probability of pit "stifling" with depth and other factors, pitting and crevice corrosion rate, pit density, and pit size as a function of exposure conditions (temperature, pH, chloride concentration) and pit depth, pitting and crevice corrosion rate in the presence of galvanic coupling with the carbon steel outer-barrier as a function of exposure conditions (temperature, pH, and chloride concentration), pit depth, and degree of the outer barrier degradation.

For MIC, the expert elicitation will provide information on the probability and spatial distribution of microbe (bacteria and/or fungi) colony population on the carbon steel outer barrier and the corrosion-resistant inner barrier, corrosion rate of carbon steel and localized (pitting/crevice) corrosion rate of the inner barrier under the microbe colony. Elicitations will be expressed as a function of the exposure conditions (temperature, relative humidity, and the contacting solution chemistry), nutrient availability, "liquid" water availability, and the presence of carbon steel and its corrosion products.

The expert elicitations, where applicable, will include associated uncertainty (and/or bounding uncertainty) and variability.

Convolution Approach to Waste Package Degradation Abstraction. As discussed previously, the approach used in TSPA-1995 to develop abstraction of the WAPDEG results included a first pit penetration distribution, and a binning of the first pit perforation history into eight discrete waste package groups. Each waste package in a particular group had the same, representative pitting perforation history after the first pit penetration. Clearly, this approach results in some averaging of the waste inventory exposure rate but is fairly easy to represent within RIP. An alternative approach (referred to as convolution approach) is described in the following. This approach attempts to reduce the need for binning of waste packages according to their failure time.

If the first pit breakthrough rate (i.e., sometimes called the package failure rate, or initial breach rate) is designated as $f(t)$, then $F(t)$ is the cumulative fraction of failed packages at time t:

$$F(t)=\int_0^t f(\eta)d\eta \tag{6.4-1}$$

where

$$\int_0^\infty F(\eta)d\eta=1$$

If N_p is the total number of packages in the inventory, then $N_pF(t)$ is the total number of failed packages at time t. Furthermore, let $g(t, \tau)$ designate the pit breakthrough rate at time t (i.e., the rate at which pits are penetrating the inner barrier at time t) for a package that failed at time τ (i.e., a package which had the first pit penetration at time τ). In general, τ will be a function of many model parameters, including waste-package design, waste-package materials, corrosion mode, and environmental variables such as temperature, relative humidity, and chemical parameters, etc., i.e., τ = τ(design, materials, corrosion mode, T, RH, pH,...). Based on these definitions, $G(t, \tau)$ is the total number of pits through a given package at time t, assuming that the first pit broke through at time τ:

$$G(t,\tau)=\int_\tau^t g(\eta,\tau)d\eta+1 \tag{6.4-2}$$

where $G(\tau, \tau) = 1$, i.e., there is one pit through the package at failure. (In reality, we could ignore the "1" in the above equation.)

Finally, we can get the total number of pits that have broken through all packages in a given group[1], at any time t, by the following convolution integral:

$$\#\text{pits}(t) = \int_0^t N_p f(\tau) G(t,\tau) d\tau \qquad (6.4\text{-}3)$$

The functions $f(t)$ and $G(t, \tau)$ will be developed in WAPDEG output in tabular form, as will the function $F(t)$ which is required for "primary container failure distribution" in RIP, and is used to compute how much waste inventory in the waste package group is exposed to the near-field environment at any given time

6.4.6 Base Case and Sensitivity Cases

The waste package degradation model for TSPA-VA is intended to be based more on mechanistic processes than in previous TSPA analyses, to incorporate additional important corrosion processes, and to be supported by additional site-specific corrosion data. Additional abstractions developed from the waste package degradation expert elicitation (WPDEE) project (M&O, 1997b) will also enhance the confidence of the waste package degradation modeling and abstraction for TSPA-VA.

The key components of the WP degradation modeling and abstraction in TSPA-VA are presented in Figure 6.4-2. This figure indicates the key processes involved in degradation of the waste package and the source of that information. The temperature, relative humidity, and in-drift water dripping across the repository will be abstracted from the thermo-hydrology modeling. The pH and chloride concentration of the dripping water and the oxygen partial pressure across the repository will be derived from the near field geochemical environment model. Information on the MIC rates for input to the waste package degradation model will be obtained from the effort in MIC modeling.

The base case waste package degradation model will be based on the WAPDEG model. Table 6.4-2 lists the important processes, parameters to be included, values for those parameters (when known), and the implementation of those values. The information in the table has been derived

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[1] "Group" in this context means a set of waste packages subject to a different thermal-chemical-hydrologic environment, and having a specific type of inventory (e.g., commercial spent fuel). Each group will require a different WAPDEG simulation, which will generate functions f, F, g, and G specific to the given group.

from the most recent process-level understanding, the current conceptualization, and the on-going WPDEE. Some of the information may be modified as the WPDEE is finalized or as additional experimental results are collected. The humid air corrosion of the outer barrier will be initiated at critical relative humidity of 70-80% for no drip conditions and 60-70% for drip conditions. Aqueous corrosion of the outer barrier will be initiated using the RH threshold of 80-100%. Aqueous corrosion of the outer barrier will also be initiated if dripping occurs. Localized corrosion of the outer barrier will be characterized by a pitting factor dependent on the pH of the incoming water. The uncertainty in these values will be captured by sampling over the specified ranges of values. The inner barrier corrosion will be initiated after corrosion has progressed through the outer barrier and will have a corrosion rate dependent on geochemistry of the contacting solution, and localized corrosion characteristics such as pit depth and pit density.

Variability in the environment from waste package to waste package will also be stochastically represented in the base case. It is expected that two thermo-hydrologic zones (center, edge) will be defined in the base case, leading to two different waste package degradation regions. Within those zones there will also be variability in the rate and episodicity of dripping on waste packages. This will be represented with certain percentages of the packages having dripping at various rates, and with certain percentages of the surface of the individual package that is dripped on. Waste packages with different waste types (such as young spent fuel, old spent fuel, and vitrified defense high-level waste) are expected to have different exposure conditions, particularly in terms of temperature, relative humidity and water dripping, which are due mostly to different heat outputs from the decay of those wastes. Degradation of those waste packages will be modeled explicitly in TSPA-VA.

For humid-air corrosion of the outer barrier, the base case potentially will include other processes such as salt-deposit effect, water dripping, humid-air corrosion at elevated temperature (there are significant kinetic responses to relative humidity at elevated temperature than ambient temperature), and critical relative-humidity threshold for the initiation of humid-air corrosion as a function of temperature and type of salt. For aqueous corrosion, additional features which may be in the model include the effect of water chemistry (especially, pH and chloride concentration), a refined temperature-dependency, and the critical relative-humidity threshold for a transition from humid-air to aqueous corrosion as a function of temperature and type of salt. Those modifications and refinements expected to be made for TSPA-VA will be supported by the site-specific data that are being developed from the comprehensive corrosion testing program underway at LLNL (McCright, 1997).

Impacts of such variability on waste-package degradation are possibly large in the potential repository. More robust approaches to represent the variability in those areas identified at the workshop are required, and more realistic methodology on how to implement those models/abstractions representing the variability into waste package degradation model should be developed.

The base case WAPDEG output will be corrosion or degradation time-histories of the waste packages for a given design and multiple repository environments, addressing the two major performance goals of waste package, i.e., waste containment and waste isolation (DOE, 1996). The waste containment goal will be measured by the time of waste package failure that is defined as first pit or crack perforation. One form of the WAPDEG output will provide the fraction of waste package corroded (# pits as f(t)) as a function of time. Each pit will be modeled as a constant size, unless additional data on this becomes available. This information gives the rate at which the waste inventory is exposed to the near-field environment, thus making the waste available for degradation and release. The waste isolation goal for the waste package could be provided by slow, gradual release of radionuclides from failed (or perforated) waste package. The other form of the WAPDEG output will describe the distribution of subsequent perforations or opening of failed waste packages as a function of time. This information provides the perforated (or opening) area of a failed waste package, through which radionuclides transport and are released.

Sensitivity Analysis. Sensitivity analyses will be conducted on numerous features of the waste package degradation base case to evaluate their importance to waste package performance. In particular, many of the abstractions provided by the WPDEE will be evaluated in a sensitivity framework. The following highlight some of the key sensitivity analyses to be conducted.

- **Patches.** Prior to determination of the base case model, the number and dimension of the patches will be evaluated. This will be determined and documented as the base case WAPDEG model.
- **Critical RH switches for corrosion.** The critical RH for initiation of humid-air and aqueous corrosion of the carbon steel outer barrier will be varied and evaluated as to it's importance in waste package degradation.
- **Pitting factor of carbon steel.** The sensitivity of waste package degradation to the pitting factor for localized variations of the outer barrier corrosion will be evaluated using different pitting factor values and their distribution.
- **Dripping rates.** The rates, frequencies, and location of drips will be stochastically varied and evaluated to determine important thresholds (if any) of this processes effect on waste package degradation.
- **Chemistry effects.** The effects of pH of the contacting solution and oxygen partial pressure on the carbon steel outer barrier corrosion, and the effects of pH and chloride concentration of the contacting solution on the corrosion-resistant inner barrier corrosion will be evaluated to determine the sensitivity of waste package degradation to these geochemical factors.
- **Galvanic protection.** The extent of galvanic protection of the inner barrier will be evaluated using different thresholds for the process. The sensitivity study will include any new experimental data collected prior to final implementation.

- **MIC.** The sensitivity of waste package degradation to the MIC effect will be evaluated using alternative MIC-enhancement factors for the outer barrier and microbe-perturbed localized water chemistry for the inner barrier corrosion.
- **Stress corrosion cracking of the inner barrier.** The effects of stress corrosion cracking of the corrosion-resistant inner barrier on waste package degradation (waste package failure and subsequent degradation) will be evaluated using a preliminary model from LLNL. Determination of the crack opening distribution will be included in the sensitivity study.
- **Ceramic coating on waste package.** An additional design option being considered is to add ceramic coating to the waste package. The sensitivity of waste package degradation to this design will be evaluated. Due to the lack of data on the expected lifetime of such a design, the evaluation will be done using expert judgement for the expected lifetimes.
- **Ceramic drip shield.** An additional design option being considered is to add a drip shield and associated backfill to the EBS. The sensitivity of waste package degradation to this design will be evaluated. Due to the lack of data on the expected lifetime of such a design, the evaluation will be done using expert judgement for the expected lifetimes.
- **Backfill.** The effect of backfill on waste package degradation will be evaluated in a sensitivity study.
- **Mechanical failure of degraded waste package by rockfall.** The effect of rockfall from thermo-mechanical process and seismic activity will be included using some preliminary models from Disruptive Events abstractions (Barnard, 1997).
- **Welds.** The effects of potential corrosion attack on welds on the outer and inner barriers will be included in the sensitivity study using enhancement factors for the barriers.

6.4.7 References

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Table 6.4-1. List of Issues Most Important to Waste Package Degradation.

Major Issue	Sub-Issue #	Sub-Issue Description
Carbon-Steel Outer-Barrier Corrosion and Salt-Scale Deposit Effect	1.11	Refluxing and concentration of electrolyte (Cl^-, pH, etc.)
	1.12	Microbiological
	1.13	Temperature dependence on corrosion
	1.18	Model of salt buildup
	1.1	Critical RH (transition from dry oxidation to humid-air corrosion)
	1.2	Critical RH (transition from humid-air to aqueous corrosion)
	1.5	Aqueous corrosion
	1.8	Flow rate and episodicity of water
	1.20	General corrosion in humid-air environment
Nickel-Based Material Inner Barrier Corrosion	2.2	Aqueous corrosion
	2.5	Crevice corrosion (geometry, etc.)
	2.21	Cathodic (or galvanic) protection
	2.25	Choice of waste package materials
	2.20	Barrier interface environment
Galvanic Coupling Effect	3.2	Barrier materials (alloy choice)
	3.10	Water chemistry vs. time
	3.5	Threshold for galvanic protection cessation
	3.4	Crevice corrosion (including welds)
	3.9	Electrode area ratio
	3.3	Ionic conductivity at interface
	3.1	Fabrication process (contact effectiveness)
	3.13	Water-contact mode inside container & outside container

Table 6.4-1 List of Issues Most Important to Waste Package Degradation (continued).

Major Issue	Sub-Issue #	Sub-Issue Description
Microbiologically Influenced Corrosion	4.1	Water variability
	4.5	Amount of nutrients
	4.13	Susceptibility of inner barrier
	4.10	Preferential weld susceptibility
	4.8	Container material (microconstituents)
Rockfall, Premature Failure, and Structural Failure	5.10	Timing of rockfall

Table 6.4-2. Base Case Parameters for Waste Package Degradation

Process	Parameter	Values	Implementation
CAM humid-air corrosion	T threshold for corrosion initiation	96-104 °C; dist. TBD	WAPDEG
	RH threshold for humid-air corrosion initiation	No drips: 70-80%; dist. TBD Drips: 60-70%; dist. TBD	WAPDEG
	Aqueous corrosion	if dripping > TBD rate	WAPDEG
	General corrosion	if pH <10, PF <1.5; dist. TBD if pH>=10, PF=1-6, mean=4;dist. TBD pit density evolution TBD	WAPDEG
CAM aqueous corrosion	RH threshold for aqueous corrosion initiation	No drips: 85-100%; dist. TBD Drips: 70-95%; dist. TBD	WAPDEG
	Aqueous corrosion	if dripping > TBD rate	WAPDEG
	General corrosion	if pH <10, PF <2; dist. TBD if pH>=10, PF=1-6, mean=4;dist. TBD pit density evolution TBD	WAPDEG
CRM corrosion	Localized corrosion	No drips: general corrosion rate TBD	WAPDEG
	Threshold for corrosion initiation	T: TBD Cl: TBD pH: TBD exposure time?: TBD	Need info from NFE model
	Rate of corrosion	f (pit depth): TBD	WAPDEG
	Pit density evolution	TBD	WAPDEG

Table 6.4-2. Base Case Parameters for Waste Package Degradation (Continued)

Process	Parameter	Values	Implementation
	Pit size evolution	TBD	
Juvenile Failure of WP	Early failure of WP's	TBD	WAPDEG
Galvanic Protection		Drips+pH>=10, galvanic protection; rate TBD Otherwise, no galvanic protection	WAPDEG delay in inner barrier corrosion
MIC		Drips+T<80°C, MIC; rate TBD Otherwise, no MIC	WAPDEG corrosion rate modifier
Mechanical failure of degraded WP		Threshold stress by rx on WP vs degradation degree; effect TBD	WAPDEG corrosion rate modifier

Note: Values generally taken from WPDEE (M&O, 1997b).

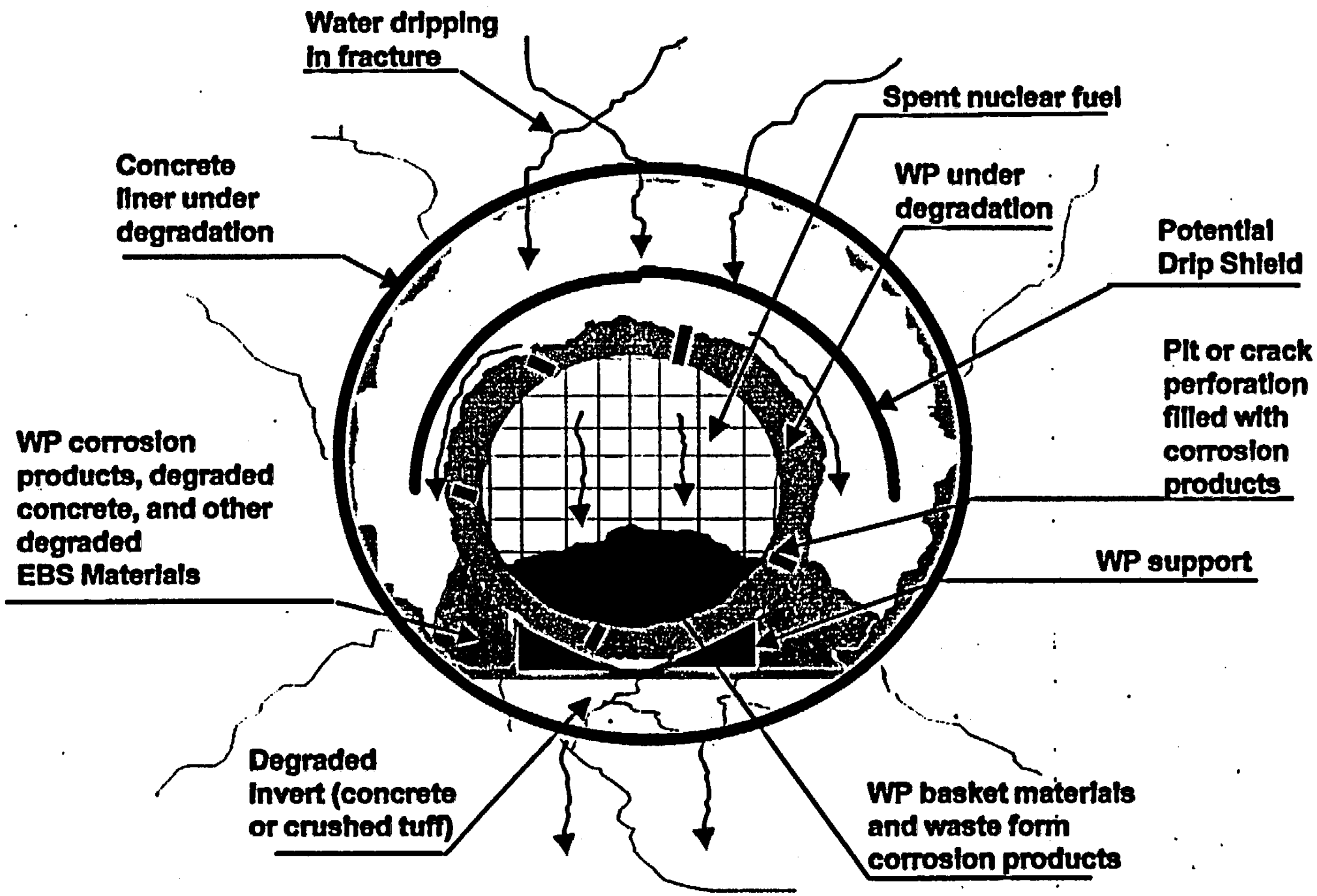

Figure 6.4-1. Schematic of Important EBS Components

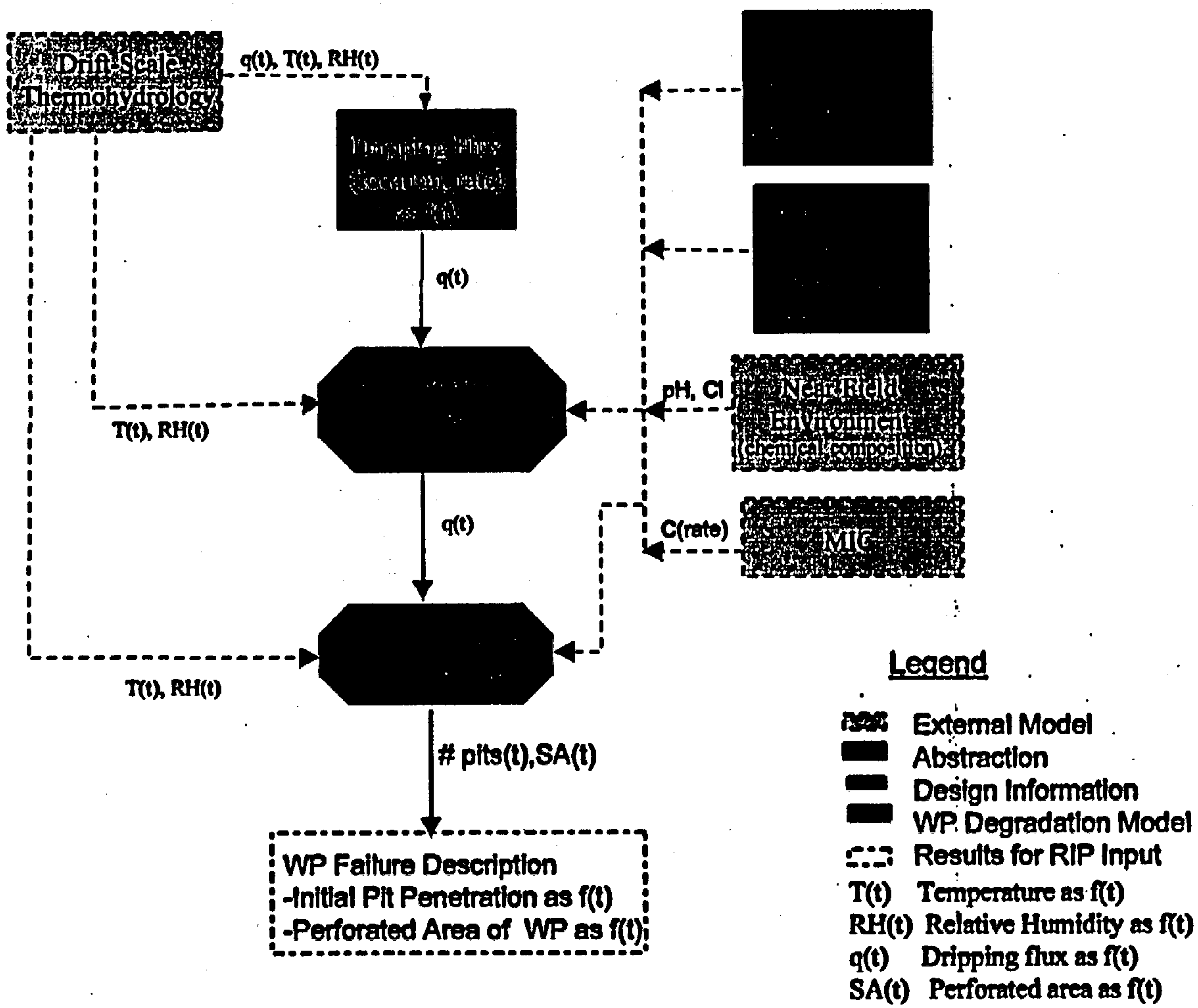

Figure 6.4-2. Schematic of Waste Package Degradation Model Information Flow

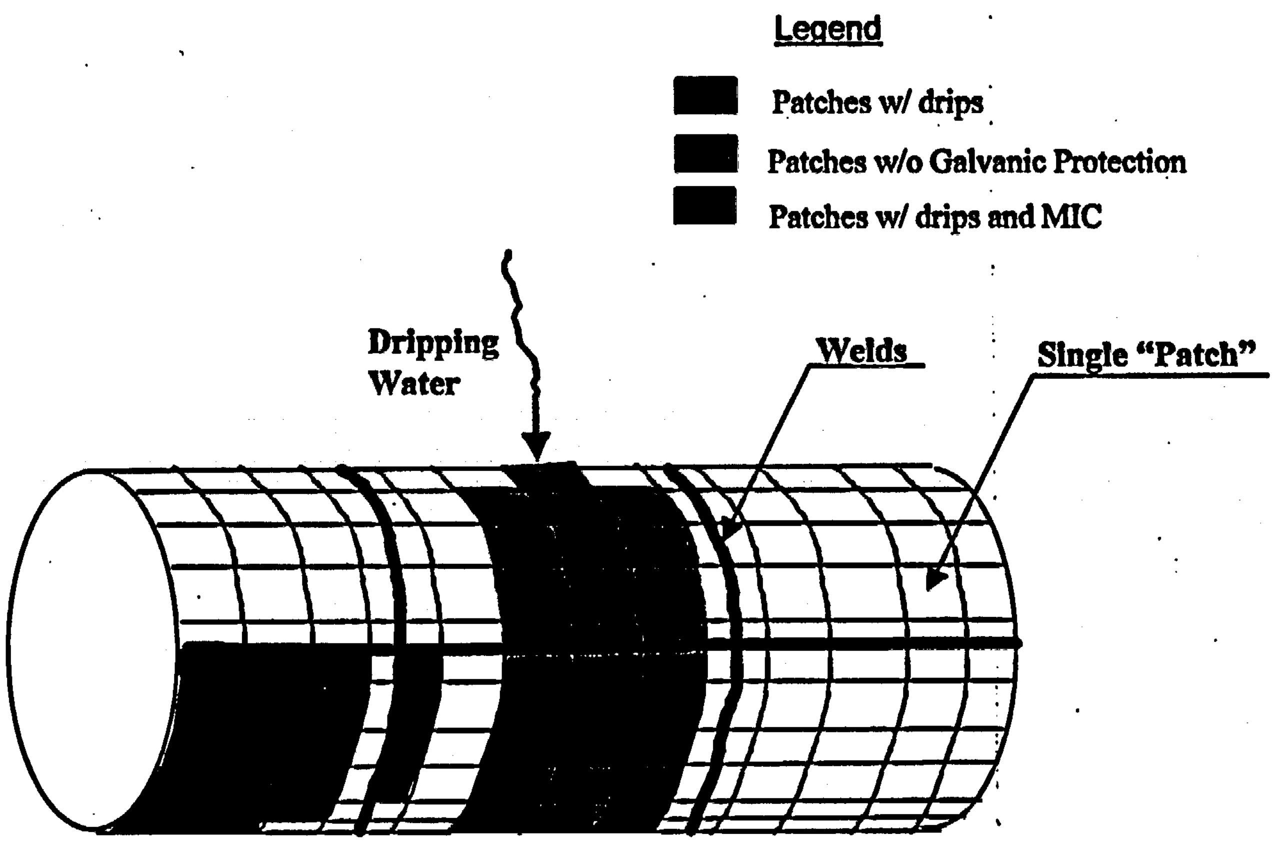

Figure 6.4-3. Schematic of the WP Degradation Conceptual Model

6.5 WASTE FORM AND CLADDING DEGRADATION

Jerry McNeish, Eric Siegmann, Steve Steward

6.5.1 Introduction

General. There are several waste forms which may be disposed of in the potential Yucca Mountain Repository, including commercial spent nuclear fuel (CSNF), defense high level waste glass (DHLW), and U.S. Department of Energy spent fuel (DOE SNF). There is considerable variability in the inventory both within and between each of these waste forms. In particular, the DOE SNF has over 250 waste form types. The expected inventory for CSNF and DHLW waste forms for 39 radionuclides is presented in Table 6.5-1. Tables 6.5-2 to 6.5-4 provide information on the grouping of DOE SNF and the inventories for 13 categories. The analyses conducted for TSPA-VA may reduce the overall number of radionuclides considered in order to capture the key contributors to dose.

The ongoing Environmental Impact Statement (EIS) analyses also include additional waste forms to be evaluated as to their effect on performance of the repository. The waste streams to be considered for the EIS include: **1) Base Case.** Total of 70,000 MTHM of waste comprised of 63,000 MTHM commercial spent nuclear fuel (CSNF), 2,600 MTHM of DOE SNF and 4,400 MTHM (equivalent) of HLW; **2) Option 1.** Base case plus an increase in CSNF up to a ceiling of 105,000 MTHM plus all existing MOX fuel, plus all DOE HLW glass logs, ceramic logs and other HLW forms that are not classified as RCRA hazardous waste. The total waste for this option is 170,000 MTHM; **3) Option 2a.** Includes Option 1 plus all additional DOE-EM items except RCRA classified hazardous wastes. This includes Pu logs, greater than class C (GTCC) waste, DOE SCW and TRU waste not meeting the WIPP acceptance criteria.; **4) Option 2b.** Includes Option 2a plus disposition of all surplus fissile material. These additional waste streams will not be incorporated into the TSPA-VA, but will be reported in the concurrent EIS document.

The waste form degradation models (rate of dissolution for CSNF and DHLW glass) in previous TSPA analyses have been based on experimental data. Functional fits to the dissolution rate data have been derived to show dependency on various state variables such as temperature, pH, and total carbonate (CO_3), which represent aggressive water chemistry. For CSNF, the dissolution model was developed as a function of total carbonate concentration, pH, and temperature. The atmospheric oxidation of CSNF to higher oxide phases can be represented primarily as a function of temperature (WFCR, V1.2). For DHLW, the degradation model was developed as a function of pH and temperature. DOE SNF has not been included in previous TSPA evaluations, but degradation/dissolution models have been developed for the current categorization of the waste forms (Duguid, et al, 1997).

No models of cladding failure have been used in previous analyses. The cladding was assumed to fail at the same time as the waste package. Also, there has been no modeling of the inner canisters for those waste form types which are packaged in this manner.

Input. The waste form and cladding degradation models require input of temperature, waste package degradation, pH, CO_3, and rate of water flux into the waste package. Figure 6.5-1 indicates the information flow for the waste form and cladding degradation models. The vertical flow into the drift, through the engineered system (drift liner, backfill, and waste package materials) prior to reaching the waste form itself will alter the ambient groundwater geochemistry and rate.

Output. The primary output from the waste form and cladding degradation model is the release of radionuclides (source term) to the next component of the engineered barrier system, either the rubblized container or the invert underlying the waste package. Another output is the effect of the waste form release on the near field environment chemistry, especially in terms of pH. This component is important to the near field and immediate far field transport altered chemistry plume below the repository, the so-called carrier plume.

6.5.2 Treatment of this Process Model in Previous TSPA's

In TSPA-1995, initial bounds on the aqueous concentration of radionuclides in ground water that has reacted with the waste form are derived from the waste form dissolution rate model. Subsequently another filter is applied which compares the dissolution-based aqueous radionuclide concentration with a solubility-limited value that is sampled from either a distribution of solubility limits for radionuclide-bearing minerals, or a functional form for the solubility limit for each radionuclide considered. If the sampled solubility-limited value is lower for a given radionuclide than its concentration derived from the waste form dissolution, then the aqueous concentration is set to the solubility-limited value and the difference in mass is calculated to "precipitate" out of solution. These solubility-limited values place constraints upon the aqueous concentration of the particular radionuclide *element* considered, with each isotope of that element present in proportion to its isotopic abundance.

In TSPA-95, the entire waste form surface area is assumed to be exposed to the near-field environment as soon as the first pit penetrates the waste package. The waste form is then assumed to be covered by a "thin" water film, and alteration processes are initiated. For DHLW glass, the dissolution rate equation is primarily a function of temperature and pH, but includes the effects of dissolved silica in the contacting solution. The current glass dissolution rate model predicts monotonically increasing dissolution rate with temperature. The radionuclides are assumed to be released as fast as the glass structure breaks down. Radionuclide release from HLW glass should also be constrained by their solubility limit. The model does not include any solution chemistry other than pH and the dissolved silica concentration. For Spent Nuclear Fuel (SNF) a semi-empirical model for intrinsic alteration rate of the spent fuel matrix was developed from the experimental data reported by Gray et al. (1992) and Steward and Gray (1994). The model was expressed as a function of temperature, total carbonate concentration, and pH of contacting water. The alteration rate apparently strongly depends on temperature and total carbonate concentration, and is less influenced by pH.

Previous TSPA analyses have not assumed any waste isolation benefit from fuel cladding or canisters interior to the waste package.

6.5.3 General Description of Process Model

Spent Fuel Dissolution Model. The input for the SNF dissolution model is the experimental data reported by Gray et al (1992), Steward and Gray (1994), and WFCR Ver. 1.2. Additional data collected by Argonne National Laboratory spent fuel dripping experiments is also being considered in this model. The dissolution rate model is currently being updated by Stout and Steward, based on non-equilibrium thermodynamics, and is expected again to provide a response surface of SNF dissolution as a f(T, pH, and [CO_3]), with the addition of spent fuel burnup as an independent variable.

Glass Dissolution Model. The input for the HLW glass dissolution model is the experimental data obtained by Finn/Bates. The major dependencies in the model are T, pH, dissolved silica. The model output will be a response surface of DHLW dissolution as a f(T, pH). AREST-CT analyses are being conducted to provide a response surface for DHLW dissolution as a f(T, pH).

Cladding Model. The objective of the cladding abstraction is to develop clad failure fractions as a function of time. Both cladding perforation and exposure mechanisms and measure of subsequent fuel surface exposure over time is needed to better assess the source term. The model assumes the cladding fails in two stages, perforation and unzipping. Perforation releases the fission gas in the cladding and exposes the fuel to oxygen if the WP and outer canister is breached.

The cladding model incorporates an improved analysis of cladding stress that accounts for burnup, surface oxidation during irradiation, and potential surface cracks. Potential perforation mechanisms being modeled are:

- creep failure,
- uniform surface oxidation,
- mechanical (rock fall , earth quake, or basket) failure.

Creep failure is modeled using Peeh's model (Peehs, 1986) although Chin's model (Chin, 1989) will be reviewed. There is some discussion as to whether or not uniform surface oxidation (in leaking WPs) will cause cladding failures itself as well as contribute to creep failure. The failure depends on time at temperature. Mechanical failure is expected to be the mechanism to terminate cladding credit because of loss of the repository geometry at later times. Cladding failure due to ZrO_2 occurs because ZrO_2 has about 2% volume increase strain. This oxide surface strain will cause compressive loading on the cladding. The rate of ZrO_2 formation is given in the WFCR (Stout, 1996). Incorporation of a model for cladding oxidation will be evaluated. Cladding failed prior to receipt at the repository will be included as a percent juvenile failure in the cladding model.

Other failure mechanisms, which have been addressed either with separate calculations or literature surveys and are not expected to be included in the abstraction, are hydride re-orientation, and microbial corrosion. Delayed hydrogen cracking (DHC) is another potential failure mechanism which may be included in the cladding model.

Many of the above mechanisms will produce small perforations in the cladding that will expose only a limited amount of fuel to the environment (mechanical failure treated separately). If the containment barriers and any additional canister is also perforated, the UO_2 fuel will be exposed to oxygen and/or water and will be able to further oxidize. Depending on which UO_x minerals are formed and how the minerals form, the fuel might expand, cracking the cladding open and exposing most of it to the environment. Two mechanisms will be modeled, dry oxidation and wet oxidation. The desired results of the cladding abstraction is the fraction of fuel exposed as a function of time for a given WP event sequence defined by PA. This quantity affects the source term in the PA.

6.5.4 Issues Associated with Process Model

The key issues from the Waste Form Degradation Workshop for four categories: 1) cladding and canister credit, 2) spent nuclear fuel dissolution, 3) SNF post-dissolution water chemistry and precipitation, and 4) DHLW glass degradation and release are presented in Table 6.5.5. Analysis plans were developed to attempt to provide useful abstractions from each of these categories.

Some issues raised at the workshop were not addressed by the abstraction/testing plans for various reasons.

1.1.1 Inventory of SNF. Assumed that this will be addressed by another part of the YMP project or existing representation will be used.

1.1.2 Distribution of radionuclides. May be incorporated in fuel model if needed and if reasonable representation is available, possible deferment to future TSPA.

2.1 Inventory of glass waste. Inventories expected from other activities, or old values will be used. TSPA-VA model will be based on one DWPF glass type.

2.2 Distribution of radionuclides. Lower priority, may be incorporated in release model when appropriate.

2.3 Canister degradation. No performance credit for DWPF canister expected in TSPA-VA. Canister credit for other wastes to be developed as appropriate.

6.5.5 Major Assumptions and Approach to Abstraction of Process Model for TSPA

Four plans were developed to address the key issues associated with modeling of waste form and cladding degradation. The plans are in the following areas: 1) cladding and canister credit, 2) spent fuel dissolution, 3) spent fuel post dissolution water chemistry and precipitated phases, and 4) DHLW glass degradation and release.

The primary objective of the cladding and canister credit plan was to develop a time dependent distribution for perforation and fuel exposure. The key hypothesis for the plan was that the cladding/canister can delay the release of radionuclides to the repository environment. The primary product from the cladding modeling is an abstraction (simple model) of clad failure fraction as a function of time, incorporating cladding perforation and exposure mechanisms and a measure of subsequent fuel surface exposure over time.

The spent fuel (SF) dissolution and alteration rates plan objective was to update a bounding spent fuel intrinsic dissolution rate model that provides an output water chemistry and feeds into the second abstraction, post-dissolution water chemistry and precipitated phase formation.

The key hypothesis for this plan is that the spent fuel intrinsic dissolution rate is the primary determinant of the aqueous release rate of highly soluble radionuclides and also the rate of spent fuel alteration into precipitates and colloidal species. The rate of change of aqueous "in solution" radionuclide release concentration is essentially the intrinsic dissolution rate times the wetted surface area (exposed by cladding failure) for quasi-steady rate processes. This product provides the source term for alteration and radionuclide transport through the unsaturated zone (UZ), and can be modeled.

The primary product to TSPA-VA is to provide SF dissolution rate model as function of temperature, burnup, and bounding, aggressive water chemistry.

Another analysis plan was developed for post-Dissolution/Release Radionuclide Concentration, Water Chemistry and Precipitated Phase Formation of Alteration Layer on Spent Fuel Surface. The objectives of this plan were to estimate radionuclide "in solution" and colloidal concentrations at the altered waste form surface by the following steps:

- To relate the alteration layer rate of formation to the intrinsic dissolution rate.
- To use the released concentrations from unsaturated test data to evaluate alteration layer retention factors for highly soluble radionuclide species that are not congruently released at a rate equivalent to ^{99}Tc.
- To use the released concentrations from unsaturated test data to estimate spent fuel alteration film concentration of "in solution" and colloidal radionuclide species.

The primary hypothesis of this plan is that the spent fuel dissolution rate for thin water films on the spent fuel surfaces rapidly reaches radionuclide concentrations that exceed their solubility limits, for most radionuclide species except ^{99}Tc. Thus the aqueous radionuclides may precipitate, forming secondary phases and radiocolloids to reduce the "in solution" radionuclide concentration to values at or near the solubility limits. Thus, the precipitation rate and the quantity of precipitates are directly proportional to the intrinsic dissolution rate (WFCR, 1996).

A secondary hypothesis is that the secondary phases (minerals) are not all ideal compounds and that these phases incorporate some radionuclide species substitutionally or interstitially (such as Sr or Cs). The rates of formation of precipitates and the incorporation of substitutional and interstitial species is unknown in detail. However, these rates can be estimated from the Argonne National Laboratory (ANL) unsaturated tests, based on radionuclide concentrations in released waters relative to ^{99}Tc concentrations. This requires a hypothesis that these tests are near a quasi-steady-state rate and the averaging of data can be performed to smooth out some sample to sample variation. With this approach, some retention factors for spent fuel radionuclide species will be estimated for alteration layer precipitates relative to the ^{99}Tc aqueous release. Finally only dominant alteration phase minerals can be identified and will be compared with mineral phases identified at natural analog sites.

The key products for TSPA-VA include:

- Solid phases - identification, radionuclide content, paragenesis, final solubility limiting phase.
- Solution - major element composition, radionuclide content, colloid content.

- Rate model relating aggregated precipitated phase formation to intrinsic dissolution rate.

The plan for abstraction of the DHLW Glass Degradation and Radionuclide Release Model has a single objective to model the alteration of DHLW glass waste and the release of radionuclides as a function of temperature, water chemistry, water contact mode and the extent of vapor hydration prior to liquid water contact.

The key hypotheses of the work are to:

- The rate of radionuclide release from DHLW will contribute to the total radionuclide mass release rate from the EBS, which is a TSPA-VA performance measure.
- Exposure of glass to humid air alters the surface of the glass sufficiently that subsequent radionuclide release must consider both altered and unaltered glass.
- The alteration and dissolution of DHLW will determine the species (aqueous, colloidal, particulate, etc.) for subsequent RN transport analyses.
- The reaction of glass will release significant amounts of non-radioactive elements, e.g. alkalis, alkaline earths, and silica that will affect the EBS and near field chemistry.

The primary products to TSPA-VA are:

- Humid air alteration: Look-up table of alteration rate (gm/m2/day) as a function of temperature and relative humidity. This will be a best estimate based on work done on early waste glass compositions.
- Aqueous alteration: Analytic expression of dissolution rate (gm/m2/day) as a function temperature, pH and silica concentration.
- Aqueous release from unaltered glass: Bounded by availability from aqueous alteration rate but not solubility limited due to colloid formation. Information can be obtained from YMP generated data, but not for Savannah River Laboratory 202 glass.
- Aqueous release from altered glass: Bounded by rapid release of a substantial amount of the altered inventory. Initially, the release is dominated by a soluble actinide fraction due to complexation of actinides with anions in the glass. Subsequently, the release is governed by the spallation of altered material from the glass and potential transport of colloids. The availability of this information is dependent of the continued support of DOE-EM for ongoing experiments that have been done outside the YMP.

Secondary Products from the plans are :

- Description of the physical and chemical nature of alteration products. Some information is available from YMP generated data, the majority is from DOE-EM.
- Characterization of aqueous and colloidal species and the radionuclide distribution in these phases. Some information is available from YMP generated data, the majority is from DOE-EM. However, YMP is currently funding investigation of waste form colloids.
- Alteration of water chemistry due to interaction with the glass. Some information is available from YMP generated data, the majority is from EM.

6.5.6 Base Case and Sensitivity Cases

The base case waste form and cladding degradation models will include specific models for each of the waste forms (i.e., CSNF, DHLW, DOE SNF, Naval Fuel) and a newly developed cladding model. The dissolution and cladding models will be used as response surfaces within RIP in the analyses. In general, after the waste package has been breached, the dissolution models will become active. The cladding model will have some early failure component, but will also provide a description of the failure of the cladding through time. These models are briefly described below.

Spent Nuclear Fuel Dissolution Model. The model for dissolution of CSNF to be used in the base case will be a response surface from the empirical model being developed by Steward (LLNL). The model will be based on existing data and will include dependencies on temperature, pH, and total carbonate (WFCR Sec. 3.4.2).

Defense High Level Waste Glass Dissolution Model. The base case representation of the DHLW glass dissolution will incorporate existing data and include dependencies on temperature and pH (Bourcier, LLNL, WFCR Sec. 3.5.2).

Cladding Model. The base case representation of the cladding model will provide a failure representation of the cladding for use in the calculations which determine the exposure of the waste form as a function of location, environment, and time. The key processes included in the cladding model base case include

- creep failure,
- uniform surface oxidation,
- mechanical (rock fall , earth quake, or basket) failure.

Creep failure is modeled using Peehs model. Other failure mechanisms which have been addressed either with separate calculations or literature surveys and will not be included in the abstraction, are hydride re-orientation, and microbial corrosion. Delayed hydrogen cracking (DHC) is another potential failure mechanism which may be included in the cladding model. Current evaluations indicate it is not an important failure mechanism (Siegmann, 1997, personal communication).

Two mechanisms will be modeled, dry oxidation and wet oxidation. The desired results of the cladding abstraction is the fraction of fuel exposed as a function of time for a given WP event sequence defined by PA. This quantity affects the source term in the PA.

The cladding model can be implemented in RIP as "secondary container failure distribution" using multiple failure modes:

- a juvenile failure percentage of the cladding which represents failure prior to receipt at the repository;
- a long-term corrosion or degradation that applies to all packages and starts at time 0 with a distribution based on expected failure as a f(t);
- a "degenerate" failure distribution which applies to a certain percentage of the packages TBD at a given time TBD. The degenerate failure is meant to represent simultaneously cladding failing for the specified percentage of packages to represent a failure mode such as basket collapse. The time at which the cladding fails degenerately could be a function of the local environment. Basket collapse time frames will be determined in separate studies by the Waste Package Development Group of the M&O.
- an additional long term failure due to mechanical failure will also be implemented.

Sensitivity cases.

Dissolution models. The dissolution rates of the waste forms are uncertain, in part due to the lack of data on such rates under various environments. The sensitivity of the release to the dissolution models will be evaluated by varying the dissolution rates. There is additional uncertainty in the dissolution model based on the evolution of the repository system. The dissolution may be dominated by incoming water chemistry or by the fuel and secondary phases.

Cladding model. Alternative to the base case, the cladding could be modeled as part of the waste form response surface; for example, as a modification of the reactive surface area. The sensitivity of the release to this model will be evaluated.

6.5.7 References

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Table 6.5.1. Inventory for TSPA-VA: CSNF and DHLW

Isotope	Commercial Fuel Inventory at 30 years (Ci/MTHM)[1]	HLW Glass Inventory at 30 yrs (Ci/MTHM)	Isotope	Commercial Fuel Inventory at 30 years (Ci/MTHM)[1]	HLW Glass Inventory at 30 yrs (Ci/MTHM)
^{227}Ac	1.84E-05	3.29E-04	^{239}Pu	3.66E+02	2.59E00
^{241}Am	3.83E+03	4.73E+01	^{240}Pu	5.40E+02	1.81E00
^{242M}Am	2.22E+01	1.13E-02	^{241}Pu	3.48E+04	8.10E+01
^{243}Am	2.53E+01	2.01E-02	^{242}Pu	2.06E00	2.75E-03
^{14}C	1.42E00	*	^{226}Ra	2.57E-06	5.13E-08
^{36}Cl [2]	1.14E-02	*	^{228}Ra	3.18E-10	*
^{244}Cm	1.19E+03	6.24E00	^{79}Se	4.53E-01	5.02E-02
^{245}Cm	3.45E-01	3.09E-05	^{151}Sm	3.62E+02	*
^{246}Cm	7.14E-02	3.50E-06	^{126}Sn	8.73E-01	*
^{135}Cs	5.27E-01	6.29E-02	^{99}Tc	1.44E+01	1.81E00
^{129}I	3.52E-02	1.04E-06	^{229}Th	3.63E-07	8.26E-06
^{93M}Nb	1.87E00	3.00E-01	^{230}Th	3.69E-04	6.78E-06
^{94}Nb	8.46E-01	1.65E-05	^{232}Th	4.47E-10	5.74E-05
^{59}Ni	2.42E00	1.48E-02	^{233}U	7.20E-05	3.19E-04
^{63}Ni	3.18E+02	*	^{234}U	1.38E00	2.74E-02
^{237}Np	4.47E-01	1.55E-02	^{235}U	1.73E-02	4.34E-05
^{231}Pa	3.39E-05	5.33E-04	^{236}U	2.79E-01	2.38E-04
^{210}Pb	6.93E-07	1.49E-08	^{238}U	3.15E-01	2.07E-03
^{107}Pd	1.29E-01	*	^{93}Zr	2.44E00	3.83E-01
^{238}Pu	3.13E+03	2.19E+02			

[1] Assumes 40,747 MTHM PWR with a burnup of 42,300 MWd/MTHM, and 22,253 MTHM BWR with a burnup of 32,250 MWd/MTHM and an age of 30 years at the time of disposal.

[2] Chlorine inventory assumed to be non-gaseous release.

* Does not exist or is present in insignificant amounts.

Table 6.5-2. Categories and Typical Members of DOE-Owned Spent Fuel

Category	Typical Spent Fuel
1. Uranium Metal	N-Reactor
2. Uranium-Zirconium Alloy	Heavy Water Component Test Reactor (HWCTR)
3. Uranium-Molybdenum Alloy	FERMI (Enrico Fermi Reactor)
4. Uranium Oxide, intact clad	Commercial Pressurized Water Reactor (PWR)
5. Uranium Oxide, failed clad	Three Mile Island (TMI) core debris
6. Uranium-Aluminum Alloy	Advanced Test Reactor (ATR)
7. Uranium Silicide	Foreign Research Reactor-Materials Test Reactor (FRR MTR)
8. Uranium-Thorium Carbide, high integrity	Fort St. Vrain
9. Uranium-Thorium Carbide, low integrity	Peach Bottom
10. Uranium or Uranium-Plutonium Carbide, non-graphite	Fast Flux Test Facility (FFTF) Carbide
11. Mixed Oxide	Fast Flux Test Facility (FFTF) Oxide
12. Uranium-Thorium Oxide	Shippingport Light Water Breeder Reactor (LWBR)
13. Uranium-Zirconium Hydride	Training Research Isotopes-General Atomics (TRIGA)

Table 6.5-3. Summary of Metric Tons Heavy Metal (MTHM) for Each Category of Spent Fuel at the DOE Sites

Category	INEEL	Savannah River	Hanford	Total
1	34.6		2102.2	2136.8
2	0.04			0.04
3	3.93			3.93
4	79.27		17.8	97.07
5	84.11	3.67	0.15	87.93
6		8.96		8.96
7		11.4		11.4
8	24.67			24.67
9	1.66			1.66
10	0.05		0.17	0.22
11	1.55		10.2	11.75
12	49.66			49.66
13	1.96		0.03	1.99

Table 6.5-4. Radionuclide Inventory for Each Category of DOE-Owned Spent Fuel

Isotope	Category 1 (Ci/MTHM)	Category 2 (Ci/MTHM)	Category 3 (Ci/MTHM)	Category 4 (Ci/MTHM)	Category 5 (Ci/MTHM)	Category 6 (Ci/MTHM)	Category 7 (Ci/MTHM)	Category 8 (Ci/MTHM)	Category 9 (Ci/MTHM)	Category 10 (Ci/MTHM)	Category 11 (Ci/MTHM)	Category 12 (Ci/MTHM)	Category 13 (Ci/MTHM)
^{227}Ac	4.75E-06	9.51E-07	1.30E-02	3.35E-04	9.47E-05	1.43E-06	2.31E-06	0.00E+00	1.02E-01	3.29E-08	4.31E-08	6.13E-01	2.87E-06
^{241}Am	2.36E+02	7.69E+01	8.26E-02	3.78E+03	7.20E+01	5.27E+01	8.41E+00	7.57E+01	9.58E+01	1.58E+04	1.47E+04	1.19E+00	1.01E+01
^{242m}Am	6.28E-03	2.33E-01	0.00E+00	5.47E+00	1.46E-01	1.71E-01	5.81E-02	2.05E-02	4.91E-02	2.75E+01	2.55E+01	1.25E-02	1.12E-01
^{243}Am	3.56E-02	7.59E-01	1.33E-09	1.73E+01	6.75E-02	4.95E-01	1.20E-02	5.41E-01	4.76E-02	0.00E+00	2.16E+00	2.38E-03	1.24E-02
^{14}C	3.15E-01	1.63E-03	4.01E+00	7.84E-02	1.11E-02	1.27E+00	3.59E+00	4.39E+00	1.35E+00	0.00E+00	2.02E-02	9.55E-01	4.26E+00
^{36}Cl	0.00E+00	0.00E+00	1.02E-02	0.00E+00	4.12E-05	3.83E-02	1.08E-01	5.51E-02	3.83E-02	0.00E+00	3.76E-04	2.13E-02	1.28E-01
^{244}Cm	9.84E-01	3.13E+01	1.24E-10	7.53E+02	2.81E+00	2.04E+01	3.37E-01	1.70E+01	1.25E+00	0.00E+00	9.08E+01	2.29E-01	3.36E-01
^{245}Cm	4.45E-04	1.60E-03	3.39E-16	2.98E-01	6.94E-04	1.04E-03	1.38E-05	2.84E-03	1.44E-04	0.00E+00	3.72E-02	4.73E-05	6.85E-06
^{246}Cm	5.89E-05	1.10E-04	1.11E-19	5.06E-02	1.11E-04	7.14E-05	9.22E-07	1.41E-03	4.69E-06	0.00E+00	6.31E-03	3.13E-06	1.92E-07
^{135}Cs	3.48E-02	1.54E+00	8.29E+00	3.17E-01	1.22E-01	1.44E+00	1.26E+00	3.52E-01	9.52E-01	0.00E+00	4.13E-02	2.87E-01	1.61E+00
^{129}I	2.86E-03	3.26E-01	2.11E-01	3.69E-02	1.73E-02	2.21E-01	3.12E-02	4.21E-02	2.64E-02	0.00E+00	4.37E-03	1.58E-02	3.62E-02
^{93m}Nb	1.67E-01	1.73E+00	8.47E+00	1.24E+00	1.43E-01	1.22E+00	2.94E-01	1.88E-01	1.67E+00	0.00E+00	1.52E-01	4.40E-01	3.54E-01
^{94}Nb	5.84E-08	3.27E-04	1.53E+00	0.00E+00	8.81E-05	6.98E-02	1.97E-01	0.00E+00	1.77E-02	0.00E+00	6.83E-04	2.22E-02	2.32E-01
^{59}Ni	1.77E-02	0.00E+00	1.26E+01	0.00E+00	8.03E-03	7.48E+00	2.11E+01	3.51E-01	5.27E-02	0.00E+00	7.34E-02	7.31E-02	2.49E+01
^{63}Ni	1.67E+00	0.00E+00	2.63E+02	3.59E+03	9.88E-01	9.20E+02	2.60E+03	8.43E+00	5.43E+00	3.35E+02	3.11E+02	8.91E+00	3.08E+03
^{237}Np	3.37E-02	4.00E+00	6.10E-01	3.62E-01	1.91E-01	2.61E+00	8.04E-02	3.31E-01	2.66E-01	1.23E-01	1.51E-01	1.01E-03	9.59E-02
^{231}Pa	1.20E-05	4.57E-05	3.67E-02	5.88E-04	1.69E-04	4.26E-05	3.71E-05	3.79E-01	1.74E-01	1.26E-07	1.65E-06	1.55E+00	4.51E-05
^{210}Pb	3.51E-11	1.72E-10	2.63E-07	7.47E-08	4.62E-08	1.19E-10	2.22E-11	9.32E-05	9.39E-06	0.00E+00	3.72E-09	1.12E-04	6.78E-11
^{107}Pd	6.49E-03	2.28E-01	2.35E-01	1.00E-01	1.57E-02	1.57E-01	2.63E-02	1.77E-02	1.72E-02	0.00E+00	1.23E-02	3.43E-03	2.99E-02

Table 6.5-4. Radionuclide Inventory for Each Category of DOE-Owened Spent Fuel (continued)

Isotope	Category 1 (Ci/MTHM)	Category 2 (Ci/MTHM)	Category 3 (Ci/MTHM)	Category 4 (Ci/MTHM)	Category 5 (Ci/MTHM)	Category 6 (Ci/MTHM)	Category 7 (Ci/MTHM)	Category 8 (Ci/MTHM)	Category 9 (Ci/MTHM)	Category 10 (Ci/MTHM)	Category 11 (Ci/MTHM)	Category 12 (Ci/MTHM)	Category 13 (Ci/MTHM)
^{238}Pu	4.73E+01	8.62E+03	3.02E+01	3.51E+03	4.11E+02	5.61E+03	1.11E+02	1.65E+03	6.63E+02	2.32E+03	2.34E+03	3.94E+00	1.06E+02
^{239}Pu	1.07E+02	2.14E+02	3.60E+03	3.87E+02	1.24E+02	2.15E+02	2.16E+02	4.58E+00	1.48E+01	1.26E+04	1.14E+04	2.55E-01	2.28E+02
^{240}Pu	6.24E+01	1.22E+02	1.11E+01	5.78E+02	4.56E+01	1.09E+02	8.41E+01	7.71E+00	1.16E+01	1.09E+04	9.86E+03	1.46E-01	8.87E+01
^{241}Pu	6.85E+02	4.20E+04	1.10E+00	3.07E+04	4.47E+03	2.90E+04	5.39E+03	0.00E+00	1.08E+03	9.09E+04	8.57E+04	3.47E+01	6.59E+03
^{242}Pu	3.01E-02	1.83E-01	6.96E-08	1.91E+00	3.69E-02	1.22E-01	1.05E-02	0.00E+00	1.53E-02	2.91E-04	2.38E-01	3.27E-04	1.22E-02
^{226}Ra	9.96E-07	4.38E-10	1.18E-06	3.11E-07	1.76E-07	3.04E-10	6.00E-11	9.90E-05	3.37E-05	1.52E-07	1.55E-07	6.43E-05	1.13E-10
^{228}Ra	8.05E-11	2.48E-11	7.50E-06	2.70E-04	7.78E-05	6.13E-08	1.73E-07	1.33E-01	8.60E-02	3.17E-11	6.61E-10	1.01E-01	1.76E-07
^{79}Se	3.90E-02	5.88E+00	3.05E+00	3.94E-01	3.01E-01	4.00E+00	5.55E-01	5.99E-01	4.86E-01	0.00E+00	4.49E-02	3.51E-01	6.46E-01
^{151}Sm	6.38E+01	5.30E+03	1.27E+04	1.13E+03	3.67E+02	3.76E+03	9.50E+02	9.18E+02	9.19E+02	9.18E+03	8.42E+03	1.29E+02	1.20E+03
^{126}Sn	6.81E-02	5.26E+00	6.96E+00	4.98E-01	2.98E-01	3.58E+00	5.16E-01	2.82E-01	4.49E-01	0.00E+00	5.83E-02	3.94E-01	5.98E-01
^{99}Tc	1.31E+00	1.98E+02	8.26E+01	1.37E+01	1.02E+01	1.35E+02	1.88E+01	1.51E+01	1.46E+01	0.00E+00	1.56E+00	3.27E+00	2.18E+01
^{229}Th	8.08E-09	2.12E-08	4.33E-06	8.03E-04	2.24E-04	3.04E-08	4.71E-08	5.65E-01	2.47E-01	3.87E-09	2.27E-08	2.60E-01	5.74E-08
^{230}Th	8.88E-07	1.71E-06	2.11E-04	5.55E-05	2.59E-05	1.14E-06	1.09E-07	3.87E-02	4.76E-03	3.34E-05	3.40E-05	9.83E-03	1.92E-07
^{232}Th	1.05E-10	4.05E-10	7.92E-06	2.85E-04	8.20E-05	1.81E-07	5.11E-07	1.03E-01	9.06E-02	5.25E-11	1.87E-09	1.20E-01	5.18E-07
^{232}U	4.97E-06	1.82E-04	1.81E-03	3.11E-01	8.56E-02	2.04E-04	2.45E-04	1.40E+02	9.45E+01	7.15E-06	1.60E-05	1.69E+02	2.81E-04
^{233}U	4.22E-01	1.71E-01	9.04E-01	2.98E-01	1.00E-01	1.13E-01	6.39E-03	1.14E+01	1.57E+01	2.30E-01	2.34E-01	8.39E+00	1.05E-02
^{234}U	1.61E-02	1.63E+00	5.86E+01	3.37E-02	1.18E-01	1.20E+00	4.05E-01	4.40E-02	2.44E-01	3.84E-04	3.71E-03	5.64E-04	4.94E-01
^{235}U	6.11E-02	6.71E+00	2.29E+00	2.82E-01	3.33E-01	4.53E+00	5.49E-01	4.33E-01	6.16E-01	6.83E-02	9.16E-02	1.16E-03	6.63E-01
^{236}U	3.32E-01	3.00E-02	2.68E+01	2.64E-01	3.15E-01	1.28E-01	3.06E-01	1.09E-03	2.55E-03	7.15E-13	3.33E-02	1.83E-05	2.91E-01
^{93}Zr	1.83E-01	3.02E+01	1.22E+01	1.85E+00	1.53E+00	2.07E+01	3.34E+00	2.19E+01	2.31E+00	0.00E+00	2.11E-01	8.21E-01	3.89E+00

Table 6.5-5. Issues From Waste Form Degradation and Mobilization Workshop

Category	Issue	
1. Cladding and Canister Credit	1.2.1	Cladding degradation model
	1.2.2	SNF Oxidation model
	2B1	Cladding and Canister Credit
2. Spent Nuclear Fuel Dissolution	1.2.3	SNF Dissolution model
	1.4	Representation of data uncertainty/variability
	1.5	Exposed SNF surface area
	2B2	Evolution of NFE
	2B3	Dissolution
3. SNF Post Dissolution Water Chemistry and Precipitated Phases	1.2.4	Time dependent evolution of solution and alteration layer
	1.3	Representation of evolution of the near-field environment
4. DHLW Glass Degradation and Release	2.4	Vapor hydration
	2.5	Dissolution rate
	2.6	Time dependent evolution of solution and alteration layer
	2.7	Evolution of NFE
	2.8	Representation of data uncertainty/variability
	2.9	Exposed glass waste surface area

Table 6.5-6. Base Case Parameters for Waste Form Degradation -- TBD

Process	Parameter	Values	Implementation
Spent Fuel Dissolution	Dissolution rate	TBD	Response surface
DHLW Dissolution	Dissolution rate	TBD	Response surface
Cladding Degradation	Fuel pin geometry Temperature history WP failure times Water chemistry on cladding	W1717WL geometry from Waste Package Design from Waste Package Degradation model from NFE geochemistry model	Response surface

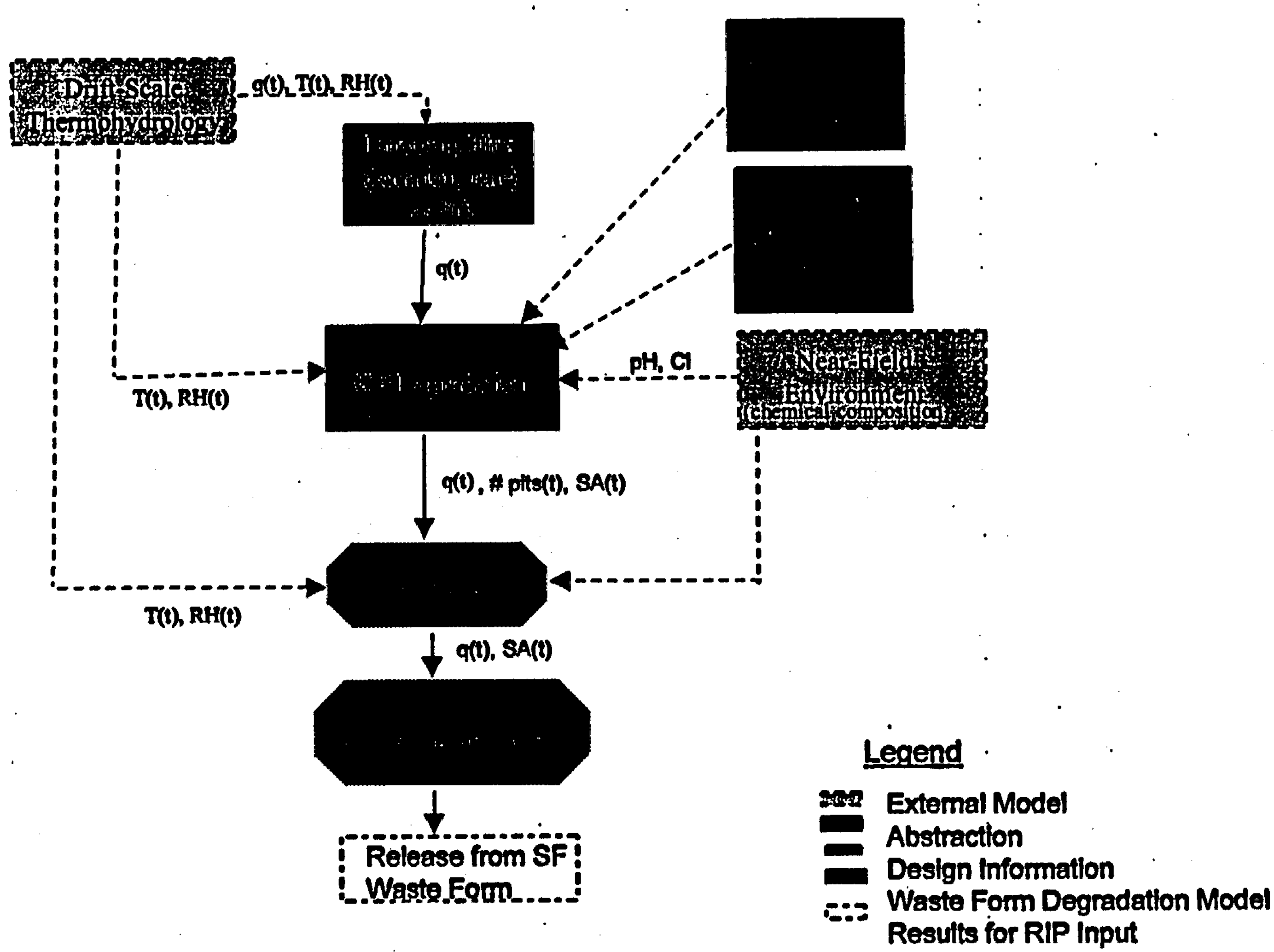

Figure 6.5-1. Schematic of SF Waste Form and Cladding Degradation Model Information Flow

6.6 ENGINEERED BARRIER SYSTEM TRANSPORT

Joon Lee, Jerry McNeish

6.6.1 Introduction

General. The engineered barrier system described herein is comprised of all of the components of the repository within the drift. The overall transport of radionuclides within the engineered barrier system (EBS) is dependent on numerous parameters and models. The transport is influenced by the waste package degradation, the waste form degradation (including cladding degradation), the thermo-hydrologic environment, the chemical environment, and the design of the EBS. The radionuclide release from the EBS is then transported to the natural system for ultimate transport through the unsaturated zone and on to the saturated zone.

The dissolution rates of the waste forms (spent nuclear fuel (SNF) and vitrified defense high-level waste (DHLW) used in TSPA-1995 (M&O, 1995) were derived from experimental data using the flow-through technique (Gray, et al., 1992; Steward and Gray, 1994; and Knauss, et al., 1990). Radionuclide concentrations mobilized from the waste form are then constrained by the solubility limit of each radionuclide. The solubility limits were formatted into distributions by expert elicitation (Gauthier, 1993). In some cases, the solubility constraints were described as a function of temperature (Am, Cm, Np, Pu), or pH (Am, Np, Pu). The solubility constraints for several radionuclides have been reevaluated in 1997. In particular, the Np solubility constraint has been updated based on additional information (Sassani, 1997). Along the transport pathways in the EBS, the radionuclide concentrations are checked against the solubility limit.

Input. The key input to the EBS transport model is the mobilization of radionuclides from the waste form. Also important are the flux and chemistry of the water moving through the system. Other transport parameters including retardation and permeability of the EBS materials (e.g., waste package, corrosion products, invert materials) also are significant inputs to the system. Figure 6.6-1 shows the information flow for the EBS transport system as it is connected to the overall system.

Output. The output from the EBS transport model is a release of radionuclides from the EBS into the geosphere, including both aqueous and gaseous release.

6.6.2 Treatment of this Process Model in Previous TSPA's

Taking into account the approaches and the conceptual models for the release from failed waste container and the EBS in TSPA-1995, both steady-state and "quasi-transient" diffusive mass transport models were developed (Lee, et al, 1996a). The term "quasi-transient" is used because the model incorporates steady-state diffusive transfer through the perforations of the "failed" waste container combined with transient diffusive mass transfer through the spherical shell of the invert (other EBS components) surrounding the waste container.

Three EBS release conceptual models were developed for TSPA-1995:

- Drips-On-Waste-Form. Assumed that after one pit penetrated a waste package, the inside of the waste package became the same as the drift environment. Advective flux through the waste package and onto the waste form was also permitted as soon as a single pit penetrated the waste package. Diffusive releases were dependent on the surface area of the waste package which was degraded or pitted through and the water film thickness on the waste form.
- Drips-On-Waste-Package. Assumed only diffusive releases out of the waste package. Advective flow remained on the surface of the waste package, and did not flow through the waste package. The corrosion products in the pits were assumed to prevent the advective or dripping water from entering the waste package (Lee, et al., 1996b)
- No Advective Transport with Capillary Barrier. This model assumed no advective flow into the drift, leading to only diffusive release from the engineered barrier system. This model could be operational if the engineered system provided for diversion of all advective flow away from the drift.

It was assumed in previous TSPAs that the interior conditions of failed (or perforated) waste packages are the same as the in-drift conditions. Previous TSPAs did not account explicitly for colloidal transport of radionuclides. The EBS release models were directly embedded into RIP in TSPA-1995.

The distributions of solubility limits used in TSPA-1995 are based primarily on an elicitation of chemical/geochemical experts held at Sandia National Laboratories on April 13, 1993 (Elicitation—Gauthier, 1993). Judgement of the expert panel was based on both empirical studies and modeling results, but did not include consideration of distributions used in the 1991 TSPA (Barnard et al., 1992). The results of the expert elicitation were reviewed in 1993 by the Solubility Working Group (SolWoG is composed primarily of project scientists conducting actinide solubility/speciation studies) which recommended only two modifications to the distributions of Np and Pu as discussed below. The assumptions behind the Elicitation's development of the distributions are: (1) the unsaturated zone water composition is between the composition of J-13 well water and that of UE_25p#1; (2) the solubility-limits will be determined by the far-field ground-water environment; (3) the environment is oxidizing; and (4) future climate changes may cause ground-water compositional changes. A number of additional sources were used to further constrain distributions of solubility limits for the radionuclides used in TSPA-1995. The elicited solubility constraints were input to RIP as stochastic distributions.

6.6.3 General Description of Process Model

The process model to be used in TSPA-VA is intended to be input directly into RIP and to make use of the compartment or cell modeling capability within RIP. The compartments within RIP are essentially mixing cells similar to a finite difference node. Each of the components in the EBS which are significant to performance will be defined as a separate RIP compartment. The compartments require definition of volume, material properties within the compartment, retardation within the compartment, and advective/diffusive linkages to other compartments.

A schematic of a limited set of compartments within the EBS as it may be represented in RIP is shown in Figure 6.6-2. The figure presents the mass location within the waste package and the potential connections to the mixing cells or compartments. Both advective and diffusive connections are possible between the various cells. In the figure, the waste cells represent the compartment for the waste form dissolution. This is underlain by the degraded waste package cell which represents the corrosion products of the waste package. The volume in this cell may change with time. The invert compartment underlies the corrosion products. In addition, there are cells which represent a diffusive release out of the package which are called water film cells. Inherent in this figure is the ability to model spatially heterogeneous dissolution of an individual waste package caused by localization of drift seepage onto a certain fraction of the total package area. This capability is part of the waste-package corrosion model and will be part of the EBS transport model. It is not yet decided whether it will be included in the TSPA-VA case, however, sensitivity analyses will be performed to evaluate its effect on EBS performance. (See also Section 7.2.2.2.)

6.6.4 Issues Associated with Process Model

The key issues associated with EBS transport are shown in Table 6.6-1. This was one of the major topics within the Waste Form Degradation and Mobilization Workshop (M&O, 1997). As such, one abstraction plan was developed to address the issues with the EBS transport model. The analysis plans will develop models for the EBS subsystems. The subsystem model analysis activities will include development of abstractions for the following areas: 1) waste package water seepage which addresses the water contact mode of a breached waste package, including water flow into and out of degraded waste package, 2) aqueous and colloidal radionuclide transport through the EBS components, and 3) radionuclide sorption along the EBS transport pathways as a function of pH and temperature. Once completed, those EBS subsystem models will be incorporated into the TSPA model (RIP).

6.6.5 Major Assumptions and Approach to Abstraction of Process Model for TSPA

As noted, the process model will be embedded into the RIP probabilistic framework in the form of simple analytical and/or semi-analytical solutions, thus requiring limited additional abstraction of an external process model. Sensitivity cases will be run within RIP to define the number and type of compartments which are required to appropriately represent the transport processes. The primary output from the model is the source term out of the EBS for use in UZ flow/transport modeling.

At the waste form degradation and mobilization workshop, an abstraction plan was developed for the Waste Package and Engineered Barrier System (EBS) Transport Model. The abstraction plan has the objective to develop EBS radionuclide source-term models and abstractions to feed the unsaturated zone (UZ) far-field transport model. The models to be developed will be incorporated into the RIP compartment model. This plan was developed prior to the receipt of the new version of RIP with its compartment models.

The key assumption for the EBS model is that transport of radionuclides from the waste form to the edge of the EBS will be controlled by the following process conditions:

- mode of water ingress into the breached waste package;
- mode of water contact with the waste form;
- transport of radionuclide through the breached waste package (including sorption); and
- interaction of dissolved radionuclide and the solution with degraded EBS materials.

The primary products from the plan to help substantiate the compartment model in TSPA-VA include, simple analytical, semi-analytical, and/or numerical models (possibly some response surfaces for certain model parameters) that capture water contact mode and radionuclide transport for three waste package conditions and two EBS flow-path elements:

- access of in-drift dripping water through pinhole perforations in the corrosion-resistant inner barrier of waste package;
- access of in-drift dripping water through large cracks or open areas of waste package (This is likely to lead to total exposure of waste form to in-drift dripping water and will be included as a sensitivity study in waste package analyses);
- concentration of soluble and colloidal radionuclides exiting the breached waste package incorporating interaction and transport through waste package corrosion products (e.g., iron oxides, oxyhydroxides and hydroxides); and

- concentration of soluble and colloidal radionuclides at the edge of the EBS incorporating interaction and transport through degraded concrete invert and other EBS materials.

The key workshop issues covered in this plan are:

3.1 Physical processes - water contact mode

3.2 Physical processes - transport paths

3.6 Mobilization - Colloids

3.7 EBS transport (aqueous Radionuclides) through waste package (including corrosion products)

3.8 EBS transport (aqueous Radionuclides) through other EBS components (invert)

3.9 EBS transport (colloidal Radionuclides) through waste package (including corrosion products)

3.10 EBS transport (colloidal Radionuclides) through other EBS components (invert)

The plan to abstract the solubility limits on dissolved radionuclides for TSPA-VA has a primary objective to derive constraints on dissolved radionuclide concentrations based on the long-term interactions with the geologic environment for use in Total System Performance Assessment (TSPA) calculations. These constraints will be arrived at by using thermochemical data and will reflect the chemical conditions of the system. To the extent feasible, the solubility limits will be determined for all environments (e.g., liner, waste package, corrosion products, invert, geologic formations below the repository).

The key assumption was that for some radionuclides, stable solid phase formation will occur over geologic time-scales and will provide an upper-bound to the dissolved radionuclide concentration.

The key products for TSPA-VA include providing either a response surface with uncertainties or a distribution of dissolved radionuclide concentrations which account for various fluid compositions and temperature effects and dissolved concentration limits.

The key workshop issues addressed include:

3.4 Chemical process - mobilization - solid dependence

3.5 Chemical process - mobilization - fluid dependence

6.6.6 Base Case and Sensitivity Cases

The base case EBS transport model will be developed using the RIP compartment model. As defined in Section 6.6-3, the model will discretize the EBS into several components. This will allow geochemical differences between components to be readily incorporated, as well as appropriately facilitating the transport from the waste form through the degrading waste package (including corrosion products) and invert. Solubility limits will also be compartment dependent to the extent feasible. Figure 6.6-2 shows this compartmentalization.

The base case parameters are presented in Table 6.6-2. The mass transfer rate models (i.e., diffusion, advection, or combination of both) will be developed for the appropriate compartment. Time-dependent protection from the waste package will be evaluated using a complete structural failure scenario at late time, when all isolation capability of the waste package will be assumed to be gone.

Sensitivity Cases. A series of sensitivity cases for EBS transport will be conducted for TSPA-VA. The following are key sensitivity analysis cases to be considered.

- **Compartments.** The discretization of the compartments representing various components of the EBS will be evaluated to determine the optimum number of compartments to appropriately capture the performance aspects of the components.
- **Diffusion coefficients.** Diffusion of radionuclides through the various EBS components will be evaluated in a sensitivity analysis.. The diffusion coefficient in tuff has been determined experimentally as a function of volumetric water content (Conca, 1996), but additional information must be gathered for the evaluation of diffusion through corrosion products and other EBS components. Lacking such information, sensitivity analyses using literature data for the various components will be performed.
- **Liquid saturation in EBS components.** The liquid saturation in the various EBS components is provided by the thermo-hydrologic modeling. This parameter has a significant effect on the release from the EBS attributable to diffusion. Sensitivity cases will be conducted for various values of liquid saturation in a range about those values calculated in the thermo-hydrologic modeling.
- **Water film thickness.** The water film thickness on the waste form is an uncertain parameter. The sensitivity of the release to this parameter will be evaluated.
- **Colloids.** Colloidal transport will be included in sensitivity analyses. Colloids will not be treated as dissolved species, but as a separate phase. This is discussed in more detail in UZ transport section.
- **Conceptual model uncertainties.** The conceptual model used for the EBS transport will be evaluated in a sensitivity study. Alternative conceptual models for the transport through the EBS will be evaluated.

- **In-drift water seepage.** In-drift water seepage rate and frequency are key parameters that could affect significantly the EBS transport rate. A series of sensitivity analyses will be conducted using varying rates and frequencies of in-drift seepage.
- **Waste package seepage.** One of the EBS release conceptual models discussed in Section 6.6.2 assumes dripping water onto a perforated waste package is diverted around the waste package (i.e., not flowing into the waste package). The conceptual model is based on the fact that perforations in the failed waste package will be filled (or "plugged") with corrosion products and other mineral precipitates, and these prevent the dripping water from flowing through the degraded waste package and from contacting the degrading waste form inside the waste package. The conceptual model is based on limited literature data (Jones and Wilde, 1987; Ramian and Nasrazadani, 1990). The mode of water contact with the waste package and waste form are also key important parameters to the EBS release rates. Sensitivity analysis will be conducted with a range of waste package seepage rates, assuming the drips on waste package EBS model.
- **Waste package failure mode.** Waste package failure modes (i.e., small pinhole perforation, hairline crack penetration, large crack opening, total structural failure, etc.) have significant impacts on the extent of water seepage into the waste package and the performance of the waste package as a diffusion barrier to radionuclide release. Sensitivity analysis will be conducted with different waste package failure modes that incorporate information developed from the waste package degradation abstractions.
- **Waste package premature failure.** There is always a possibility of a small number of waste packages failing prematurely. This could be caused by a number of reasons that include manufacturing defects, materials defects, damage to waste package during transportation and handling, and damage by rockfalls. Premature (or juvenile) failure of waste package, although the number is expected to be small, could have a substantial impact on the initial release rates from the failed waste package. If a waste package fails prematurely during early hot periods, the waste form inside the waste package will undergo degradation by oxidation in dry or slightly humid environments. This type of waste form degradation would lead to mobilization of radionuclides from the waste form, but radionuclides would not transport because of limited transport pathways, thus resulting in accumulation of radionuclides on the waste form. When the exposure conditions become wetter due to increased humidity and/or water seepage into the waste package, there may be a pulse-like release of radionuclides from the waste package, particularly from radionuclides that are highly soluble and mobile. A series of sensitivity analyses will be conducted for a range of waste packages that fail prematurely, the time for the failure, and exposure conditions at the failure and following the failure.
- **EBS material sorption properties.** Sorptive properties (various types of adsorption and desorption) of radionuclides on the degraded EBS materials inside and around waste package could have significant impacts on the transport behaviors of the radionuclides. There are several types of well-known isotherms to describe adsorption behaviors of adsorbate, which are dependant on the type of adsorbate and adsorbent and

the solution composition (including pH and other competing species). The sorption behaviors are also strongly affected by temperature. Sensitivity analysis will be conducted using appropriate sorption isotherms and a range of the sorption parameters in the isotherms. For example, a range of adsorption coefficients could be employed for a simple reversible, linear adsorption isotherm.

6.6.7 References

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Table 6.6-1. Issues for EBS Transport and Release

Category	Issue
1. EBS Transport and Release	3.1 Physical processes - water contact mode 3.2 Physical processes - transport paths 3.6 Mobilization - Colloids 3.7 EBS transport aqueous through WP (includes corrosion products 3.8 EBS transport aqueous - through other EBS (invert) 3.9 EBS transport - colloid - through WP (includes corrosion products) 3.10 EBS transport - colloid - through other EBS (invert)
5. Solubility Limits	3.3 Chemical processes - mobilization temp dependence 3.4 Chemical processes - mobilization - solid dependence 3.5 Chemical processes - mobilization - fluid dependence

Table 6.6-2. Reference Case for EBS Transport and Release

Process	Parameter	Values	Implementation
WP/EBS design	WP length	5.34 m	WP design
	WP diameter	1.65 m	WP design
	WP inner barrier thickness	2 cm	WP design
	WP outer barrier thickness	10 cm	WP design
	Invert thickness	1.0 m	Repository design
WP/EBS materials	WP inner barrier material	Alloy 625	WP design
	WP outer barrier material	Carbon steel	WP design
	Invert material	Precast concrete	Repository design
In-drift water dripping	Rate of water dripping, f(t, location)	TBD	Drift-scale T-H model
	Frequency of water dripping, f(t, location)	TBD	Drift-scale T-H model; EBS transport abstraction
	Location of water dripping, f(t)	TBD	Drift-scale T-H model; EBS transport abstraction
Waste package water seepage	Rate of in-drift water dripping, f(t)	TBD	Drift-scale T-H model
	WP perforation rate, f(t)	TBD	WP degradation abstraction
	WP degradation mode	TBD	WP degradation abstraction
	Rate of water seepage, f(t)	TBD	EBS transport abstraction
	Hydraulic conductivity of corrosion products in perforations	TBD	Literature
	Porosity of corrosion products in perforations	TBD (between 0.4-0.67)	Literature
Chemistry of incoming water	pH, CO3, SiO2	TBD	NFGE abstraction

Table 6.6-2. Reference Case for EBS Transport and Release (Continued)

Process	Parameter	Values	Implementation
Waste form degradation	SF degradation rate, f(T, pH, CO3)	SF degradation model	WF abstraction
	DHLW degradation rate, f(T, pH, SiO2)	DHLW degradation model	WF abstraction
Diffusive transport through perforated waste package	RN concentrations at WF surface	TBD (solubility limited RNs; alteration-limited RNs)	EBS transport abstraction
	Sorption of RNs in degraded WF and WP	TBD	EBS transport abstraction
	Number of perforations	TBD	WP degradation abstraction
	Perforation size (pit diameter, crack opening, etc.)	TBD	WP degradation abstraction
	Perforation length	TBD (2-10 cm?)	WP degradation abstraction
	Porosity of corrosion products in perforations	TBD (0.4-0.6?)	Literature
	Liquid saturation of corrosion products in perforations	TBD (estimate from NFE RH and T?)	Drift-scale T-H model
	Diffusion coefficient in perforations filled with corrosion products	Conca's model, f(volumetric	EBS transport abstraction
Diffusive transport through carbon steel corrosion products and degraded concrete in the vicinity of the WP	Porosity of the degraded materials	(0.4-0.7?)	EBS transport abstraction
	Liquid saturation of the degraded materials	TBD (estimate from NFE RH and T?)	Drift-scale T-H model
	Diffusion coefficient of RNs in the degraded materials	Conca's model, f(volumetric water content)	EBS transport abstraction
	Sorption of RNs in the degraded materials	TBD	EBS transport abstraction

Table 6.6-2. Reference Case for EBS Transport and Release (Continued)

Process	Parameter	Values	Implementation
Diffusive transport through invert	Porosity of degrading precast concrete	TBD (0.1-0.4?)	EBS transport abstraction
	Liquid saturation of degrading precast concrete	TBD	Drift-scale T-H model
	Diffusion coefficient of RNs in degrading precast concrete	Conca's model, f(volumetric water content)	EBS transport abstraction
	Sorption of RNs in degrading precast concrete	TBD	EBS transport abstraction
Advective transport around perforated WP	Rate of water dripping onto WP, f(t, location)	TBD	Drift-scale T-H model
	Frequency of water dripping onto WP, f(t, location)	TBD	Drift-scale T-H model; EBS transport abstraction
	Thickness of water film flow	TBD	EBS transport abstraction
Advective transport through carbon steel corrosion products and degraded concrete in the vicinity of the WP	Rate of advective flow in the degraded materials, f(t)	TBD	EBS transport abstraction
	Porosity of the degraded materials	(0.4-0.7?)	EBS transport abstraction
	Hydraulic conductivity of the degraded materials	TBD	EBS transport abstraction
Advective transport through invert	Rate of advective flow in degrading precast concrete, f(t)	TBD	EBS transport abstraction
	Porosity of degrading precast concrete	(0.4-0.7?)	EBS transport abstraction
	Hydraulic conductivity of degrading precast concrete	TBD	EBS transport abstraction

Note: Solubility limits and sorption coefficients will be applied to all compartments in the model.

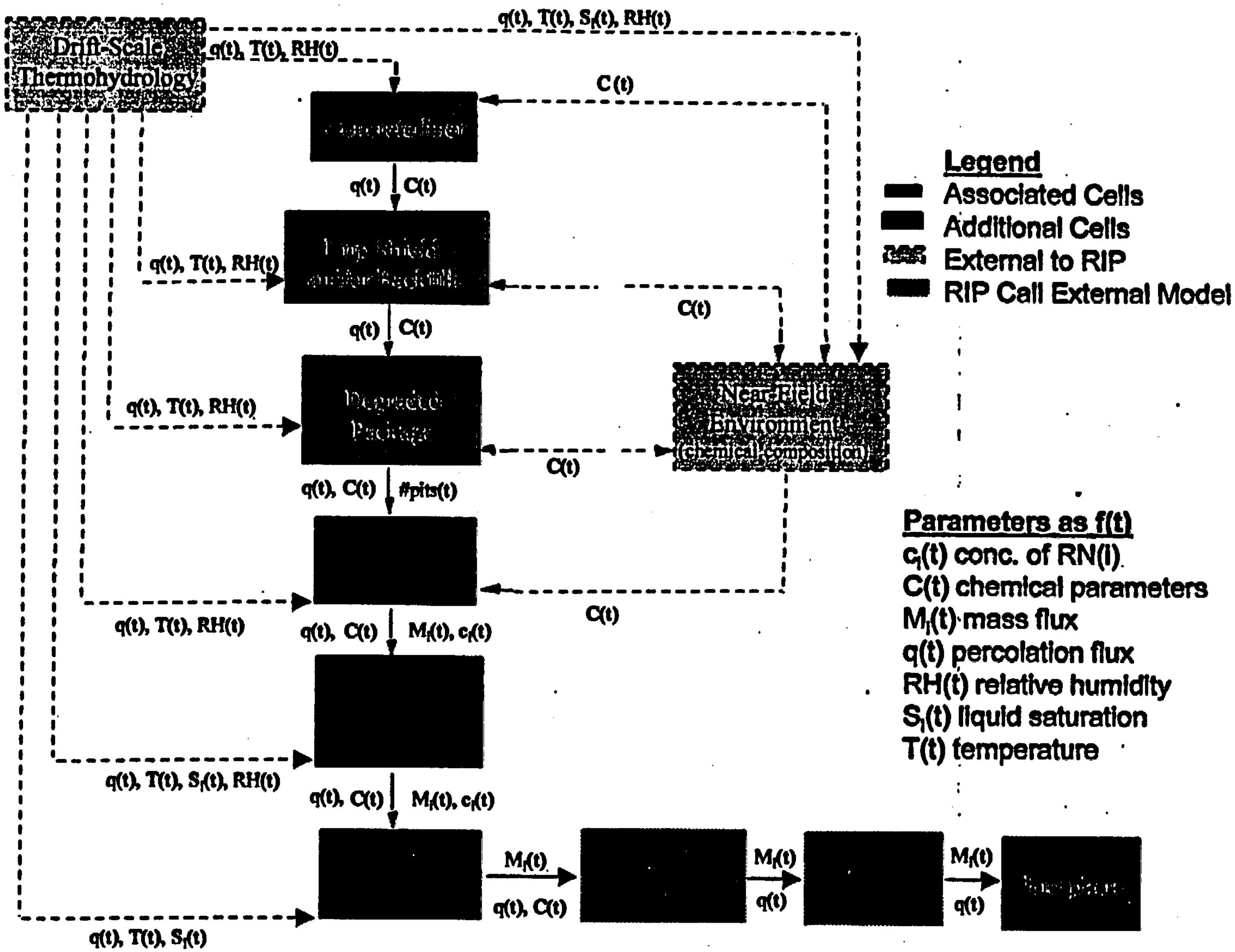

Figure 6.6-1. Information Flow in EBS for TSPA-VA

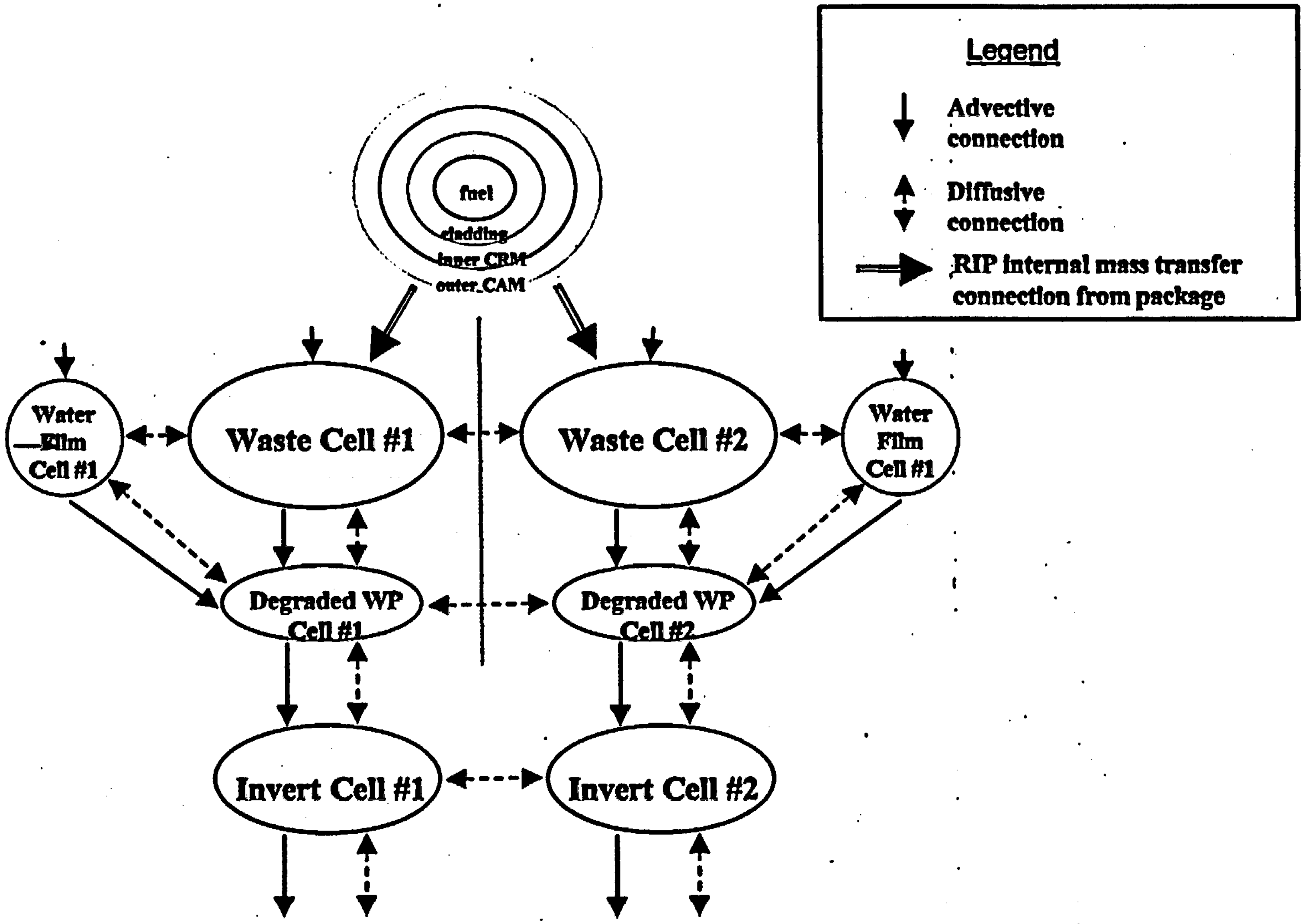

Figure 6.6-2. Schematic of EBS Transport Implemented in RIP

6.7 UNSATURATED-ZONE RADIONUCLIDE TRANSPORT

S. David Sevougian, James E. Houseworth

6.7.1 Introduction

General. Because of the relatively slow flow of liquid through the approximately 350 m of unsaturated rock beneath the potential repository, and the potential for those rocks to sorb most of the radionuclides escaping the engineered barrier system, radionuclide transport through the unsaturated zone has always been considered a key component of the natural barrier system. The primary processes affecting unsaturated zone radionuclide transport (UZRT) are radionuclide decay, advection of the bulk fluid (which transports both solutes and colloids at the liquid pore velocity), diffusion within the liquid phase, and partitioning to other phases, particularly the stationary solid or mineral phases. Because of the importance of bulk fluid advection, all of the processes affecting UZ flow likewise affect UZ transport. Therefore, all of the writeup in Section 6.1 is applicable to this section as well. Furthermore, through their effect on UZ flow and reaction rates, the thermohydrologic models discussed in Section 6.2 are likewise applicable.

In past TSPAs, UZ transport parameters found to have a major impact on overall system performance are the (1) UZ percolation rate, (2) the partitioning of flow (and thereby radionuclides) between rock matrix and fractures, and the (3) distribution coefficients (K_ds) between liquid and tuff matrix. The various radionuclide K_ds are a very significant contributor to the natural system performance in that they cause very long time retardation to the travel time of almost all the radionuclides released from the EBS. However, there are a few radionuclides that are not noticeably retarded through interaction with the host rock (such as ^{99}Tc, ^{129}I, and ^{36}Cl) and these become the most important contributors to peak dose at the accessible environment. Also, there is one radionuclide, ^{237}Np, that is only slightly sorbing to the host rock, and because of its relatively low solubility it tends to be released from the EBS over much longer periods of time than ^{99}Tc and ^{129}I, and therefore in past TSPAs it has dominated long-time releases. This has made ^{237}Np the focus of much investigation within the UZRT models. Another radionuclide of potential significance to UZRT is ^{239}Pu because of the possibility of transport in colloidal form. This method of transport has not been investigated in past TSPAs, but as discussed below, will be the focus of sensitivity studies in TSPA-VA.

Input. Key inputs to the UZRT model include (1) the far-field percolation flux through rock matrix and fractures over the entire spatial domain beneath the repository and extending to the water table, and over the entire time period from breach of the waste packages out to 1,000,000 years postclosure of the repository;[2] (2) rock-water interaction parameters, generally represented

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[2] According to the National Research Council (1995), based on geologic considerations this is the longest reasonable time period for assessing performance of a repository.

as K_ds (linear, infinite-capacity sorption model), which includes the effect of all types of rock-water interactions, such as sorption, ion-exchange, surface-complexation, precipitation/dissolution, and colloidal interactions/transport; (3) dispersive parameters, such as longitudinal velocity dispersion and matrix-fracture diffusion coefficients; (4) fracture/matrix interflow from the UZ flow model; and (5) source-term strength as defined by the mass flux of radionuclides leaving the emplacement drifts. These various inputs indicate the importance of coupling the UZRT model to the various other system models, which is discussed in more detail below.

Output. The output from the TSPA-VA UZRT model will be the mass flux of radionuclides leaving the unsaturated zone and entering the water table as a function of time and location.

Following is a discussion of how the UZRT model couples to other component models of TSPA-VA (from M&O, 1997):

Unsaturated-Zone Flow. Decoupling of UZRT and UZ flow is discussed in more detail in Section 7.2.1.1. It is made possible by the assumption of a steady-state flow field, or a sequence of step changes in the flow field that reach steady state rapidly with respect to the travel time of radionuclides in the UZ.[3] As mentioned above, all parts of the unsaturated-zone flow model affect the unsaturated-zone transport model through the advective term in the transport equations. Thus, an important part of the UZ flow model with regard to UZRT is the definition of appropriate base-case hydrogeologic parameters, boundary conditions, and conceptual flow models. As discussed in Section 6.1, the base case flow model will encompass a range of these parameters based upon the dual permeability formulation.

Thermohydrology. Through its effect on the flow field and the reaction thermodynamics/kinetics, the thermohydrology model can potentially have a significant effect on unsaturated-zone radionuclide transport. These effects may be both temporary and permanent. They may be temporary through vapor/liquid movement caused by boiling and through reversible chemical reactions. They may be permanent through irreversible changes to the mineralogy and permeability of the far-field tuffaceous rock matrix and fractures. Refer to Section 6.2.5 for specific assumptions about the effects of thermohydrology on radionuclide transport, as modeled in TSPA-VA.

Waste Form Mobilization/EBS Transport. Waste form mobilization and EBS transport define the radionuclide fluxes at the emplacement drift boundary, which represent the source term for the far-field UZRT calculations. This source term is expected to provide radionuclide fluxes at the emplacement drift boundary that will vary as a function of both location within the potential

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[3] As discussed in Section 6.1 and later in this section, transient-flow studies are ongoing to check the appropriateness of this assumption.

repository and time. Feedback mechanisms, in which unsaturated zone radionuclide transport may affect waste form mobilization, have not been identified.

Saturated Zone Radionuclide Transport. The radionuclide fluxes calculated at the water table due to UZRT are a source term for saturated zone radionuclide transport calculations. This source term is expected to provide radionuclide fluxes at the water table that will vary as a function of position on the water table and time. Although no feedback mechanisms have been identified between saturated zone radionuclide transport and unsaturated zone radionuclide transport, the position of the water table is recognized as a feedback from saturated zone flow to unsaturated zone radionuclide transport.

Criticality. The possibility of a critical configuration of fissile material being assembled after release from the waste packages is referred to as external criticality. Because of the greater transport distances and the longer time available for dispersive processes, criticality in the unsaturated zone is considered much less likely than criticality in the EBS. Nevertheless, UZRT processes are being considered to evaluate the remote possibility of criticality in the unsaturated zone.

6.7.2 Treatment in Previous TSPAs

Unsaturated-zone transport has been dealt with in a number of ways in past TSPAs. In TSPA-1995 (M&O, 1995a), the Markovian algorithm in the RIP TSPA code was used (Golder, 1994). This algorithm assumes a random transitioning of radionuclide particles between fractures and matrix according to user-specified Poisson-process transition rate. Within either the fracture or matrix flow mode, the particles move by plug flow and may be retarded according to a equilibrium K_d sorption model. Velocities and fluxes in both the fractures and matrix were derived from the site process-level hydrology model using the TOUGH2 code (Wittwer et al., 1995; Bodvarsson and Bandurraga, 1996). Exact details of the TSPA-1995 UZ transport model are given in Section 7.4 of M&O (1995a). Since the RIP transport model is more of a descriptive model than a process-based model, the validity of the Markovian transport algorithm must be established by comparing breakthrough times from the RIP code over a range of parameter and model uncertainties to breakthrough times (to the water table) from the 3-D site-scale UZ transport model (Robinson et al., 1995; Robinson et al., 1996).

The RIP4.05a model used TSPA-1995 is based on a phenomenological approach that attempts to describe rather than explain the transport system (see Section 7.2). The resulting transport algorithm is based on a network of user-defined *pathways*. The pathways may be used for both flow balance and radionuclide transport purposes, and may account for either gas or liquid phase transport. The purpose of a pathway is to represent large-scale heterogeneity of the hydrologic system, such as geologic structures and formation-scale hydrostratigraphy. Fracture/matrix exchange at stratigraphic unit boundaries is also modeled in RIP405a, and is based on the total proportion of the flow that is flowing within each of the two downstream flow modes. RIP405a does not contain an abstraction for exchange due to matrix diffusion. Dispersion is not explicitly modeled in the dual flow-mode model, however the fracture/matrix interaction process does cause longitudinal dispersion of radionuclides (which may or may not follow a Fickian description). Linear adsorption for radionuclide matrix or fracture transport may be included in RIP calculations by adjusting the radionuclide velocities according to the appropriate retardation factor. For TSPA-1995 (M&O, 1995a), retardation factors were employed for certain radionuclides and rock types (different stratigraphic layers) for matrix transport, but radionuclides were assumed to not adsorb during fracture transport.

The TSPA-1995 calculations performed with RIP assumed one-dimensional transport through a set of six columns. Five stratigraphic layers were used to represent the variations in rock type between the potential repository and the water table. These variations were based primarily on the degree of welding found in the volcanic tuffs that comprise the unsaturated zone. The six columns were used to approximate the areal variations in stratigraphy and distance to the water table throughout the potential repository. A separate unsaturated zone steady flow model abstraction was used to define the steady flow in fractures and matrix between the potential repository and the water table (M&O, 1995a).

The assumption of one-dimensional transport in RIP was investigated for a limited set of conditions. Calculations of arrival time at the water table using the TOUGH2 unsaturated flow process model and a detailed two-dimensional cross-section from the USGS site-scale model were compared with stochastic RIP calculations to investigate the one-dimensional approximation used in RIP (M&O, 1995a). The results of this comparison indicated that the range of results obtained from one-dimensional transport calculations in RIP using stochastic sampling of hydrogeologic and transport properties and infiltration rates bracketed the results found by the process model.

The intra-unit fracture matrix model in RIP is based on a random Markov process for transitioning particles between the fracture and matrix continua. The primary model parameter is an empirical interaction parameter called the Poisson transition rate. To help set this parameter, comparison calculations between RIP and FEHM were conducted. FEHM (LANL, 1997) is a process-level model for unsaturated flow and transport that solves the basic differential conservation equations for unsaturated flow and transport. The conservation equations used by FEHM describe physical and chemical mechanisms that affect transport with a dual-continuum option for modeling fractured, porous rock. Chemical interactions are limited to a selection of different equilibrium adsorption models. FEHM has been used to qualitatively calibrate the fracture/matrix exchange coefficient in RIP (M&O, 1995a). A sensitivity study was also performed using FEHM that considered the relation of the fracture/matrix exchange coefficient in RIP and the more fundamental physical processes captured in FEHM (M&O, 1995b). Although matrix diffusion was not modeled in TSPA-1995, simulations with FEHM indicated that matrix diffusion can greatly delay transport through the unsaturated zone (M&O, 1995b). For TSPA-VA, there are no plans to used the RIP Markov-process transport model.

In one TSPA-1993 (Andrews et al., 1994), the Markovian algorithm was also used. In the other TSPA-1993 (Wilson et al., 1994), as well as TSPA-1991 (Barnard et al., 1992), a one-dimensional, dual-continuum model of solute transport was used. The model is implemented in the TRANS module of the computer program TOSPAC and is described in detail in Dudley et al. (1988) and Gauthier et al. (1992). TRANS was used to calculate transport in both the UZ and SZ for the ECM-flow cases. With the Weeps model, TRANS was only used in the SZ; transport in the UZ was assumed to be rapid and complete, and the source output was introduced directly into the SZ. WEEPS is a model abstraction used to represent fracture-only flow and transport.

TRANS solves two generalized advection-dispersion equations simultaneously, one for solute transport in the matrix, the other for transport in the fractures. The equations include an advective term, a term for diffusion and hydrodynamic dispersion, a term for radionuclide decay and production, a source term, and a term specifying transfer between the matrix and fracture continua. The equations are modified to disallow hydrodynamic dispersion upstream from an internal source region. Radionuclide decay chains can be accounted for. Transport of sorbing radionuclides is modeled using the linear K_d approximation. The transfer term describes both advective and diffusive coupling between the matrix and fractures. The transfer term also includes a factor to represent the matrix/fracture coupling strength (for example, to mimic fracture coatings), but this factor has only been varied in recent calculations, and not in TSPA-1991 or TSPA-1993. TRANS calculates the concentration of each radionuclide in time and space, the cumulative amount of each radionuclide that crosses each boundary, and the dose that would result from drinking the water at a given location.

6.7.3 General Description of UZ Radionuclide Transport and Corresponding Process Model

The present understanding of potential radionuclide transport in the unsaturated zone at Yucca Mountain is based primarily on the following:

- observations of present-day chemical and isotopic compositions of matrix water, perched water, infiltrating water, and saturated zone water;
- observations of present-day mineral distributions;
- laboratory experiments of radionuclide diffusion, sorption, and transport;
- numerical modeling of transport in the UZ;
- field measurements and numerical modeling used to develop an understanding of UZ transport.

Field observations of aqueous composition have been made through samples from boreholes and from the ESF tunnel. These observations include major-ion components such as chloride, sulfate, and bicarbonate, as well as environmental isotopes such as chlorine-36, carbon-14, and tritium. Observations of mineral distributions in the UZ from boreholes and within the ESF provide qualitative evidence for transport pathways. The aqueous compositional and isotopic data and mineral distribution data are used to help constrain conceptual models for UZ transport.

Laboratory experiments provide quantitative information for transport modeling on the radionuclide sorption capacity as a function of rock-type. Similarly, quantitative information for transport modeling is provided by laboratory experiments that measure the effective diffusion coefficient through rock matrix as a function of rock type and other conditions. Laboratory experiments of radionuclide migration through rock matrix and fractures provide data on the combined effects of advection, diffusion, and sorption for different radionuclides and rock types.

A numerical model for transport in the unsaturated zone is being developed at Los Alamos National Laboratory (LANL) by Bruce Robinson and co-workers (Robinson et al., 1996; Robinson et al., 1997). The numerical model is based on mathematical models of transport processes in the UZ and constrained by the observations and data discussed above, as well as the information developed for the UZ flow model. As with the UZ flow model, the available information constraining the UZ transport model is not sufficient to define a single, unique model. Therefore, performance assessment calculations of UZ transport will have to consider these uncertainties by investigating the effects of flow and transport parameter ranges and alternate conceptual models. Parameter ranges for UZ flow processes in the UZ transport model are obtained from the UZ flow model (Bodvarsson et al., 1997). Information on radionuclide sorption and diffusion are obtained from laboratory experiments (Robinson et al., 1996; Triay et al., 1996), and LANL's mineralogic model is used to define the spatial distribution of sorptive rock types (Bish et al., 1996). Alternative conceptual models for transport are discussed in Section 6.7.5, and include transient versus steady-state flow, imbedded fine-scale heterogeneities, colloidal transport, and coupled thermal models (see Section 6.2.5 for a discussion of thermal effects).

The computer code used for these calculations is called Finite Element Heat and Mass Transfer (FEHM) code (LANL, 1997). The current implementation of FEHM for Yucca Mountain employs a dual-permeability transport conceptual model of fractured rock in which transport through a fracture continuum and a matrix continuum are coupled by advective and diffusive exchange mechanisms. The model also treats sorptive interactions between radionuclides and rock, and radionuclide chain decay processes. The solution to the governing transport equations is found numerically using either a finite element approximation (with either fully coupled reactive transport or a K_d-type approach) or a particle tracking method (with the K_d approach for rock/water interactions) that is particularly efficient for advective-dominated transport problems. (The particle-tracking method will be used for TSPA-VA—see Section 7.2.2.3). FEHM calculations of the spatial distributions of environmental isotopes have been used to compare the transport model against field data.

6.7.4 Issues Associated with the Process Model

The key issues associated with unsaturated-zone radionuclide transport were compiled into four major categories for the purposes of discussion at the three-day abstraction/testing workshop held on March 5-7, 1997: physical transport processes, chemical interactions and repository-perturbed environment, heterogeneity, and model calibration. (The last category, "model calibration", was originally only an issue, but was made into a separate category during the workshop itself, in order that a small group of scientists could work on a separate analysis plan for it.) For each of these categories, the major issues identified prior to and during the workshop are listed in tabular form below, along with the relative ranking of importance assigned to them by the experts participating in the workshop. Abstraction analyses plans were then developed at the workshop (and refined thereafter) for each of the four major categories (with more than one plan for some categories), and these will form the basis for representing UZ transport in the TSPA-VA model. These abstraction approaches are discussed in detail in the next section. Tables 6.7-1 to 6.7-4 list the UZRT issues discussed at the workshop. More detail on these issues and their representation in the abstractions may be found in M&O (1997).

The overall importance ranking (see M&O, 1997) for the issues in Tables 6.7-1 to 6.7-4 were based on four criteria. These criteria were developed so that issues would be ranked against their potential effects on long-term performance. The primary effect of unsaturated zone transport on long-term performance is through the spatial and temporal distributions of radionuclide travel time to the water table and radionuclide mass flux at the water table. Travel time is potentially important for meeting requirements linked to specific time frames, whereas mass flux is a principle factor affecting dose. Although travel time and flux are linked through the water flux, these factors can vary independently. The other components of travel time and mass flux are radionuclide velocity and concentration. Therefore the four criteria chosen for ranking the issues were radionuclide concentration, radionuclide velocity, water flux, and the distribution of travel times to the water table. Model calibration was a single issue with its own category, so there are no rankings associated with it.

The abstraction approaches discussed in the next section address ten of the issues listed in Tables 6.7-1 to 6.7-4. However, the remaining issues not directly addressed in the abstractions are being investigated, in terms of flow, under work plans associated with the unsaturated zone flow and thermohydrology workshops, or as deliverables under existing workscopes. More detail is given in M&O (1997).

6.7.5 Major Assumptions and TSPA-VA Abstraction Approach

The major assumptions currently planned for the UZRT model are (depending on the outcome of the analysis plans):

- All assumptions derived from the UZ flow model (see Section 6.1), including dual-continuum flow/transport, quasi-steady-state flow (or a sequence of steady states), and no small-scale heterogeneities.
- Interphase (solid-aqueous-colloids) chemical interactions involving radionuclides may be represented with a linear K_d model(s); this includes radionuclide transport as solute species or colloidal species.
- Advection-dominated flow (i.e., high Peclet number), which allows the use of the particle tracker model.

In order to test the validity of these assumptions, the issues listed in Section 6.7.4 have been combined into five primary abstraction plans: fracture/matrix interaction parameters, transient flow and transport, colloid-facilitated radionuclide transport model, sorption models, and fine-scale heterogeneity and dispersion. As will be evident when reviewing these five plans, they primarily take the form of sensitivity and bounding analyses to demonstrate that the proposed model for UZRT in TSPA-VA adequately captures the effects of these various processes. In particular, the abstraction studies are not designed to develop response surfaces, since the planned method for modeling UZRT in TSPA-VA is to directly couple the FEHM particle tracker (LANL, 1997) in either 3-D or 2-D to the RIP V5.x executive driver as an external function call. This will utilize predetermined steady-state flow fields from TOUGH2 simulations with the UZ flow model (see Section 6.1). Thus, the abstraction plans are more for determining parameter ranges over which to run the model. However, there are other issues, too, such as a study to determine whether a colloid model should be included in the particle tracker and whether the current discretization of the spatial domain (numerical grid) is adequate.

Fracture/Matrix Interaction. Sensitivity studies investigating the effects of fracture/matrix interaction on unsaturated zone radionuclide transport will be conducted. This will be used to provide input on the significance of fracture/matrix interaction for unsaturated zone transport under differing transport conditions, and the parameter ranges that are important to capture in TSPA in order to minimize the number of performance assessment calculations.

The parameter sensitivities to be investigated are the matrix sorption parameter (K_d), fracture sorption parameter, (K_a), and matrix diffusion coefficient (D_d) within each unit. Variations in the flow field will be investigated through variations in infiltration and the fracture/matrix interaction parameter. The transport calculations will be performed using particle tracking in FEHM (LANL, 1997) for sorbing (^{237}Np) and nonsorbing (^{99}Tc) radionuclides. The radionuclide source term will be spatially distributed throughout the potential waste emplacement drifts represented in the model. The sensitivity calculations will be performed for cases in which the radionuclide inventory is released over 1000, 10,000, and 100,000 years.

Comparisons between 3-D and 2-D models will be made for base-case infiltration and the fracture/matrix interaction parameters. This will allow us to determine if 2-D cross-sections can adequately represent the 3-D behavior. Breakthrough curves and peak mass flux at the water table will be used to compare the results of different transport calculations. Relationships between the chemical transport parameters, peak mass flux value, and the time to peak mass will be developed. This may be done in the form of a response surface between the various parameters and peak mass flux and time of peak mass flux arrival.

Transient Flow and Transport. This analysis plan will consider an abstraction approach for treating the effects of transient flow and transport due to the longer-term effects of climate change or the shorter-term effects of episodic infiltration.

The abstraction approach for the longer-term transient case approximates the flow field as series of steady flow fields under varying infiltration rates. These steady flow fields are then used to for the transport calculation. A quasi-steady flow field throughout the UZ is assumed to respond instantaneously to step changes in infiltration rate. This analysis will be carried out using the 2-D site-scale model for simulations of unsaturated zone flow and radionuclide transport with longer-term transient flow resulting from the effects of climate change on infiltration. The calculations will be performed using FEHM (LANL, 1997) in dual permeability mode without the effects of repository heating. A spatially variable infiltration rate that is scaled temporally will be used as the upper boundary condition. Temporal scaling of the infiltration rate will be based on coupled climate change/infiltration models (see Section 6.1.6). Sensitivities will be conducted by varying the initial infiltration rate between 1 and 10 mm/year. The simulations will be run for time periods of 10,000 to 1,000,000 years to evaluate the effect of the quasi-steady state assumption on postclosure performance. A quasi-steady flow field that responds instantaneously to changes in infiltration rate will be tested as a model abstraction for simplifying and bounding the effects of fully transient flow and transport. The lateral boundaries will be modeled as impermeable to flow and transport. The lower boundary is defined by the water table. Both the present water table and 100 m above the present day water table (under wetter future climates) will be used. The ranges of radionuclide release rates from the potential repository will be based on TSPA-95 analyses (M&O, 1995a), unless additional information is available. The calculations will consider sorbing (^{237}Np) and nonsorbing (^{99}Tc) radionuclides.

An abstraction method for episodic transient flow and transport is being developed based on a one-dimensional fracture flow with limited matrix interaction. The transient flow and transport through fractures is assumed to be on a short time scale relative to matrix flow and transport. Simplified solutions are possible if individual episodic flow and transport events are assumed to have only a small effect on matrix saturations and radionuclide concentrations. The long-term effects of episodic flow and transport on performance may be calculated as the integrated effects of a series of individual events over the time frame of interest.

Colloid-Facilitated Radionuclide Transport. The discussion here has much in common with a similar colloid study plan in Section 6.4. It is likely that both the near-field environment objectives and UZRT objectives will be satisfied by the same analysis plan, with a slightly different focus for each area—source term and mobilization for the NFGE and far-field transport for UZRT. The objective of this analysis plan is to assess the role of colloids in facilitating radionuclide transport, and if significant, attempt to provide a model abstraction for TSPA-VA, probably coupled directly into the FEHM particle tracker. The focus of the colloidal transport analysis will be Pu colloids. Plutonium colloids are known to exist and have been observed to migrate large distances in the subsurface.

Two flow/transport models will be tested: a one-dimensional, Weeps-like (Wilson et al., 1994; M&O, 1996) calculation in which fracture transport of colloids is unaffected by matrix interactions; and a detailed, two-dimensional transport calculation using FEHM (LANL, 1997). The detailed flow and transport models will use base-case hydrogeologic parameters and boundary conditions from the site-scale UZ flow model (Bodvarsson et al., 1997). Special conditions for colloid transport, such as restricting colloid transport to fractures, will be developed and included in the transport model. Pu will be tracked in four forms: Pu in solution (in the groundwater); Pu sorbed onto host rock minerals (matrix and fracture); intrinsic Pu colloids (e.g., Pu hydrous-oxide polymers); and Pu pseudocolloids formed by the interaction of either Pu (aq) with nonradioactive colloids or Pu (intrinsic colloid) with nonradioactive colloids.

To simulate sorption on pseudocolloids, forward and reverse rate constants will be used. These parameters will be estimated, considering the available sorption sites on colloids. The concentration of nonradioactive colloids (based on stability arguments and limited measurements), estimates for forward and backward rate constants for Pu sorption onto nonradioactive colloids, and sorption information for interaction of Pu with host rock will also be provided. Stability information is available for some colloids, including iron oxides, clays, and silica. This sensitivity analysis will be performed using iron oxide as the nonradioactive colloid. The source term for Pu concentrations in solution and as intrinsic colloids will be developed, as well as an estimate of Pu associated with iron oxides in the engineered barrier system.

Sorption Models for Radionuclide Transport. The objective of this analysis plan is to assess the effects of using a linear K_d model, versus more complex sorption models, on radionuclide transport through the unsaturated zone. The K_d model has been utilized for previous TSPA calculations (Wilson et al., 1994; M&O, 1995a) and within the site-scale UZ transport model (Robinson et al., 1996). However, more complete documentation is needed to support the model abstraction that a linear K_d model bounds the effects of more complex chemical interactions that are known to occur between radionuclides and rock.

Relatively simple arguments are available to demonstrate that the use of a linear K_d model bounds the possible effects of nonlinear isotherms such as Freundlich and Langmuir. Furthermore, existing work using ion exchange and reactive transport modeling with FEHM may be sufficient to demonstrate that the linear K_d model is reasonable and conservative abstraction for chemical interactions between radionuclides and rock. Therefore, existing work will be reviewed and summarized to see if further analysis on this subject is warranted (Triay et al., 1996; Robinson et al., 1996).

Effects of Dispersion and Fine-Scale Heterogeneity on Radionuclide Transport. The objective of this analysis plan is to test the impact of fine-scale heterogeneous mineral distributions and physical dispersion on models on radionuclide transport. This modeling effort will help define the relative importance to travel times and peak concentrations of these fine-scale features, and whether effective medium properties in large-scale grid blocks are adequate.

Flow and transport calculations will use the base-case UZ flow parameters and boundary conditions and base-case transport properties in a 2-D model domain. The hydrogeologic model domain may consist of a relatively narrow cross-section that includes a few waste emplacement drifts. A no-flow/transport lateral boundary condition will be used. If this boundary condition is perceived to strongly bias the results, then a narrow section of finer spatial discretization between the potential repository and the water table embedded in a coarse-grid model may be a useful alternative. Either approach will allow for higher-resolution gridding to capture fine-scale heterogeneity and to more accurately represent physical dispersion. Heterogeneous property distributions will be derived from information available from the 3-D mineralogic model (Bish et al., 1996) combined with geostatistical realizations. Comparisons with the coarse-gridded model will be made. The model will be used to simulate transport for nonsorbing (^{99}Tc) and poorly sorbing (^{237}Np) species. The radionuclide source term will be spatially distributed throughout the potential waste emplacement drifts represented in the model. The sensitivity calculations will be performed for cases in which the radionuclide inventory is released over 1000, 10,000, and 100,000 years. Breakthrough curves for conservative (^{99}Tc) and poorly sorbing (^{237}Np) radionuclides can be used to distinguish the effects on transport. The distribution of mean travel time for alternative representations of the heterogeneous case will be compared with each other and homogeneous stratigraphic case.

Coupling of FEHM and RIP. As described in Section 6.7.2, RIP is more of a descriptive code than a process-based model. It more or less represents what has already been determined based on the detailed process-level models and codes, which in the case of the unsaturated zone would be TOUGH2 for fluid flow (Bodvarsson et al., 1997) and FEHM for flow and radionuclide transport (Robinson et al., 1996). In TSPA-1995, hydrologic simulations of UZ flow were conducted with TOUGH2 in 1-D (with confirmatory analyses in 2-D), and then the resulting fracture and matrix fluxes from TOUGH2 were abstracted into RIP. The various UZ flow abstractions were of several types (see Section 7.2.1.2). For example, coarser discretization of the hydrogeologic units was used in RIP, which required some averaging of the greater number of TOUGH2 hydrogeologic units. Also, in TSPA-1995, many 1-D TOUGH2 runs (on a representative column in the center of the repository) were conducted as a function of uncertainty in the flow parameters. The results of these multiple 1-D runs were represented as a "wide-band distribution" of matrix/fracture fluxes and velocities as a function of the uncertain infiltration rate. (The spread in the wide-band distribution at a given infiltration rate was due to property uncertainty and heterogeneity—see M&O, 1995a.) This wide-band distribution was sampled probabilistically (uniformly) in RIP.

Also, as already mentioned in Section 6.7.2, the transport in TSPA-1995 was represented using the RIP Markovian algorithm for interaction between matrix and fractures in a given hydrogeologic unit. This is again a descriptive model rather than a process model—a descriptive model that must be "verified" against the process model. Also, all the UZ flow and transport in TSPA-1995 was represented with a set of six parallel 1-D vertical columns that covered the repository area and went from the repository horizon to the water table. (This type of vertical geometric/dimensionality abstraction neglected lateral flow, although this could have been included in a descriptive fashion in RIP if the process models had been sufficiently developed at the time.)

Because the above types of flow and transport abstractions are not particularly transparent (and appear to be quite removed from the process models) and because the NRC has had reservations about the Markovian approach, a different UZ transport model is being planned for TSPA-VA. Instead of making the sorts of abstractions described above, which also require extensive postprocessing of process-model results (e.g., TOUGH2 flow fields) in order to input them into RIP pathways, we have decided to couple the FEHM particle tracker directly to RIP and model UZ transport using the 3-D site-scale LANL transport model, based on 3-D flow fields generated by the TOUGH2 LBNL site-scale flow model. This is more like the approach for TSPA-1993 (Wilson et al., 1994) which used a flow/transport process model (1-D) directly embedded into the TSPA probabilistic code. (It still may turn out that 3-D flow simulations require too much computer time, which would necessitate using a 2-D version of the particle tracker instead.)

This method should make it is easier to explain and justify the results, since the TSPA models will be more directly derived from the process models. However, run times will be much longer than with the RIP pathways algorithm, and computer memory requirements will be quite large (between 256 MB and 512 MB per process). Thus, at this writing, it still remains to be seen if it is feasible to run hundreds of realizations. If it is not, there is a new alternative in RIP V5.x compared to the old RIP V4.x used for TSPA-1995. This is the "cells" option, which allows the use of a string of adjacent finite difference cells to represent UZ and/or SZ transport along a 1-D flowpath. This alternative is more process-based than the Markovian "pipe" algorithm (as it is now called), and has less numerical dispersion than the pipe algorithm. And it can also be used to represent fracture/matrix interaction through diffusive connections between strings of parallel cells.

There is nothing inherently "wrong" with the cells approach or even the Markovian pipe approach, per se. They will run much faster, but they require more justification to external reviewers to prove that they accurately represent the physical processes. However, we feel it is more transparent to couple the process model directly with RIP, though it requires longer computation time and more computational resources.

6.7.6 Base Case and Sensitivity Cases

The base-case UZ radionuclide transport for TSPA-VA uses the base-case LBNL UZ-flow model (Bodvarsson et al., 1997) and the base-case transport parameters being developed by LANL for use in FEHM (Robinson et al., 1996; Robinson et al., 1997). The base-case transport model uses a dual-permeability flow and transport formulation with advective and diffusive fracture/matrix interaction, linear sorption in the matrix, and radionuclide chain decay. Additionally, the base case transport model will use the particle-tracking method for a two and/or three-dimensional system and steady unsaturated flow. The base case will also include the parameter variations identified for the UZ flow base case, with the remainder of the parameter ranges to be identified in the sensitivity calculations mentioned in Sections 6.1.5 and 6.7.5.

The sensitivity calculations are to address the following items (which were already discussed in some detail in the previous section with respect to the abstraction plans):

- Transport calculations to investigate sensitivities to matrix sorption, fracture sorption, and matrix diffusion, as well as variations in the flow field due to changes in infiltration and the fracture/matrix interaction parameter. (The performance measure will be mass-flux entering the water table.) Variations in the fracture/matrix interaction parameter, including various flow and saturation weighting schemes for this parameter, address the effects of different microscopic flow geometries through fractures (such as rivulets) in which the fracture/matrix contact area is restricted. Additional sensitivity calculations will also consider the effects of variations in fracture porosity and van Genuchten alpha and beta parameters. Early sensitivity results suggest that radionuclide transport is not very sensitive to fracture alpha. These sensitivity calculations will be performed using FEHM for sorbing (^{237}Np) and nonsorbing (^{99}Tc) radionuclides. The radionuclide source term will be spatially distributed throughout the potential waste emplacement drifts represented in the model. The sensitivity calculations will be performed for cases in which the radionuclide inventory is released over 1000, 10,000, and 100,000 years.

- Given a steady-flow base case, model abstractions for transient flow and transport are being investigated for two time scales: long-term transient flow/transport that results from the effects of climate change and short-term transient flow/transport due to the episodic nature of infiltration at the site surface. An abstraction for longer-term transient flow and transport under development uses a quasi-steady flow approximation. For this abstraction, a quasi-steady flow field is assumed to respond instantaneously to changes in infiltration rate to the existing steady-flow field. Therefore, transport in a time series of steady-flow fields may be used to approximate the fully transient flow and transport. An abstraction for shorter-term, episodic, transient flow and transport under development uses one-dimensional flow and transport with limited fracture/matrix interaction. The transient flow and transport through fractures is assumed to be on a short time scale relative to matrix flow and transport. With limited coupling, simplified solutions for flow and transport in the two continua are possible.

- Radionuclide transport may be enhanced by sorption onto natural or introduced colloids, or by transport of radiocolloids. The effects of colloidal interactions on radionuclide transport are being examined for Pu, which is the element most likely to show these effects. The objective is to assess the effect of colloids on the breakthrough curve at the water table (both the shape and peak height), and if significant, provide a model abstraction for TSPA-VA. One proposed abstraction (Robinson et al., 1997) treats sorptive colloidal interactions in a way that could easily be combined with the existing UZ transport model used for dissolved species. It uses a K_d approach that models colloid-solute interaction as a linear reversible sorption reaction.

- The base-case transport model uses a linear sorption model to bound the effects of more complex sorption and other chemical effects on transport. Relatively simple arguments are available to demonstrate that the use of a linear sorption model bounds the possible effects of nonlinear isotherms such as Freundlich and Langmuir. Furthermore, existing work using ion exchange and reactive transport modeling for ^{237}Np with FEHM suggests that the linear sorption model is a reasonable and conservative abstraction for chemical interactions between radionuclides and rock. Further evaluations of the linear sorption model are being investigated. Some sensitivity cases (or possibly even the base case) may include a functional dependence of the ^{237}Np K_d on some compositional parameters derived from the near-field model, such as pH and CO_3^{2-} concentration.

- The base-case stratigraphy assumes homogeneous properties within the different hydrogeologic units. The existence of finer-scale property variations within hydrogeologic units may affect radionuclide transport. In particular, the finer-scale variations of hydrogeologic properties and mineral distributions may affect advective transport and the degree of contact between radionuclides and sorptive minerals. This sensitivity study will help define the relative importance of these fine-scale features on unsaturated zone radionuclide transport and the potential use of effective properties and modifications to the physical dispersion coefficients.

6.7.7 References

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Table 6.7-1. Issues Associated with Physical Transport Processes

Issue	Issue #
What conceptual model should be used for fracture/matrix interactions?	1.1
How should long-term transient flow be included in UZRT modeling?	1.4
What range and dependencies should be used for the fracture/matrix interaction parameter?	1.2
What are the key fracture and matrix properties to consider (i.e., fracture porosity)?	1.7
How should short term transients be included in UZRT modeling?	1.3
Do we expect lateral dispersion to be important to UZRT? Can a smeared source term be used?	1.6
Do we expect longitudinal dispersion within fractures and/or matrix to be important for UZRT if fracture/matrix exchange is explicitly modeled?	1.5

Table 6.7-2. Issues Associated with Chemical Interactions and Repository-Perturbed Environment

Issue	Issue #
Is the minimum Kd approach an appropriate modeling approach for UZRT?	2.3
Do we expect colloids to play an important role in UZRT?	2.1
Do we expect thermal-chemical alteration of existing minerals to be important for UZRT?	2.5
Do we expect aqueous geochemical evolution due to the repository to be important for UZRT?	2.6
Do we expect adsorption in fractures to be important to UZRT?	2.4
Do we expect thermohydrologic/mechanical effects on flow to be important for UZRT?	2.7
Do we expect natural geochemical evolution to be important to UZRT?	2.8

Table 6.7-3. Issues Associated with Heterogeneity

Issue	Issue #
Do we expect lateral diversion of radionuclide pathways to be important for UZRT?	3.1
Do we expect that a more detailed stratigraphy (than the TSw, TSv, CHnv, CHnz, PPn) below the repository to be important for UZRT?	3.4
Do we expect areal variations in abundance and composition of zeolites to be important for UZRT?	3.5
Spatial distribution of infiltration	3.9
Are 1,2, or 3-D models needed for modeling the effects of areal heterogeneity on UZRT? (Does the dimensionality of the models for areal heterogeneity affect performance?)	3.6
How should the stratigraphy (and flow field) above the repository be treated for UZRT models?	3.3

6.8 SATURATED ZONE FLOW AND TRANSPORT

Bill W. Arnold, John H. Gauthier

6.8.1 Introduction

The saturated zone (SZ) at Yucca Mountain is the region below the water table where rock pores and fractures are completely saturated with groundwater. The SZ underlies the unsaturated zone (UZ), which contains the potential repository. Radionuclides escaping a repository, in a dissolved or colloidal form, are expected to travel through the UZ to the SZ, where they could eventually be a source of contamination for the biosphere (see Section 6.9).

Here we look at how radionuclides could migrate in the SZ to the biosphere. First, we must understand the groundwater flow system in the region, and in the vicinity of Yucca Mountain, and downgradient (downstream) to points of existing and possible future human habitation. Next, we need to understand what processes influence radionuclide transport in this flow system, in particular diffusion, dispersion, and geochemical retardation. Finally, we must look at the connection between the SZ (part of the geosphere) and the biosphere, be it via wells, evapotranspiration areas, or (in a future climate) springs and marshes.

6.8.2 Previous TSPA Modeling

Initial TSPA efforts (Sinnock, Lin, and Brannen, 1984; Barnard and Dockery, 1991) gave only cursory attention to the SZ, primarily because the anticipated regulation at the time (EPA, 1985) used a metric of cumulative releases of radionuclides across a boundary located 5 km from the potential repository; this distance was deemed insufficient to provide much delay beyond that estimated to be provided by the UZ, thus negating any need for an in-depth look at the SZ. Results of simplified modeling at the time suggested that travel times in the SZ were on the order of hundreds of years.

For TSPA-1991 (Barnard, et al., 1992), a 2-D model of the SZ was constructed based on 2-D modeling of Czarnecki (1985) and Czarnecki and Waddell (1984). The model encompassed the controlled area around the repository—the 5 km distance between the repository and the accessible environment. Boundary conditions were taken from the Czarnecki model. A particle-tracking method was implemented to determine travel times (and velocities) from the repository to the accessible environment. Particles were placed in the repository "footprint" (the area in the SZ immediately below the repository boundary) and travel times to the 5-km boundary were determined; differences in initial position and path taken produced a distribution of travel times. In general, transport was in a southeasterly direction with travel times varying between 900 and 1500 yr (velocities of 3.25 to 5.7 m/yr), and a mean travel time of about 1200 yr. The results of the 2-D model were abstracted for the TSPA calculations into a 1-D, horizontal flow tube in a single porous medium. Dispersivities were assumed to be log-uniformly distributed between 50 and 500 m. Porosity was set to 17.5%.

For TSPA-1993 (Wilson, et al., 1994), a 3-D model was constructed for the express purpose of determining whether three-dimensions were necessary to properly define the SZ. The analysis concluded that incorporation of 3-D geologic structures was necessary to match observed hydraulic heads (water-table heights) and these structures to a large degree determined the direction and velocity of groundwater flow.

The TSPA-1993 model covered a region 8 km by 8 km by 200 m below the water table. Geologic units were extrapolated at a 6-degree tilt downward through the region, based on the interpretation of geology at the water table in Fridrich et al. (1994). The system was modeled as a confined aquifer. Two conceptual models of how the large hydraulic gradient to the northwest of the site influences flow were investigated: the diversionary model, where part of the flow is drained out the bottom of the domain (presumably into the underlying carbonate strata), and the non-diversionary model, where flow only proceeds laterally through the domain. To achieve an acceptable calibration, both conceptual models required additional structures around the flat hydraulic gradient underlying the repository area. The Solitario Canyon fault and the Drill Hole Wash fault were added to the domain as low-permeability features. Acceptable calibration could be achieved only by reducing the permeability of these structures relative to other volcanic units.

Travel times and velocities were determined by calculating the transport to a 5-km "fence" of a conservative tracer from various selected locations in each of the three geologic units that intersected the repository footprint. Porosity was set to 20%. Results showed significant variability. Travel times for the various conceptual models and transport paths ranged from 230 to 1700 yr (velocities of 3 to 22 m/yr), with averages ranging from 500 to 800 yr (average velocities of 6 to 10 m/yr).

For the actual TSPA-1993 calculations, the 3-D-model results were used as input to a 1-D, single porosity model. For the Andrews et al., 1994 analysis, dispersivity was set to 500 m. For the Wilson et al. analysis, 1994, dispersivity was assumed to be uniformly distributed between 100 and 500 m. The latter analysis estimated dilution by estimating the cross-sectional area of transport plume at the boundary to the accessible environment; the estimate was based on assumed transverse dispersivities and mixing depths, and ranged between 34,000 and 2,200,000 m^2. Climate change was only approximated by water-table rise: Wilson et al. assumed a uniform distribution between 50 and 120 m.

For TSPA-1995 (M&O, 1995), velocities from the TSPA-1993 3-D model were used. A dispersivity of 500 m was assumed, along with various dilution factors for the transport path, and in some calculations for mixing with other groundwater basins, and for mixing with uncontaminated water during well withdrawal. Water table rise assumed a uniform distribution between 0 and 80 m.

TSPA-1993 and TSPA-1995 both found repository performance to be sensitive to variability and uncertainty in saturated-zone parameters. In particular, results were sensitive to parameters influencing radionuclide dilution in groundwater. In the models, these parameters were the groundwater flux, the cross-sectional flow area of the contaminant plume, and the dilution factor. In reality, the parameters correspond to the flux, matrix diffusion, dispersion (longitudinal and transverse), transport path length, well-withdrawal effects, and sub-basin mixing.

6.8.3 General Description of the Hydrogeologic System

Groundwater flow in the SZ below and downgradient of the potential repository at Yucca Mountain occurs in fractured volcanic rocks at relatively shallow depths beneath the water table, in fractured carbonate rocks of Paleozoic age at much greater depths, and in alluvium (as well as the deep Paleozoic carbonates) at distances of greater than 10 to 20 km from the repository. The hydraulic gradient indicates that groundwater flow is generally to the south and east near the potential repository, probably transitioning to more southerly flow farther to the south (Ervin et al., 1994; Winograd and Thordarson, 1975). Groundwater flow from beneath Yucca Mountain would probably be discharged to pumping wells in the Amargosa Desert given present water use conditions in the region (F. D'Agnese, oral communication). Under pre-development conditions and present climatic conditions the ultimate discharge of groundwater from beneath Yucca Mountain probably occurs at Franklin Lake Playa and/or at springs in Death Valley (Czarnecki, 1990; F. D'Agnese, oral communication).

The SZ flow system at Yucca Mountain is in the Alkali Flat-Furnace Creek groundwater Sebastian within the Death Valley groundwater flow system (D'Agnese et al., 1997) (see Figure 6.8-1). The Alkali Flat-Furnace Creek groundwater Sebastian receives recharge from within its boundaries as well as some underflow from adjoining subbasins. Recharge occurs primarily as infiltration in upland areas in the northern part of the Sebastian and from Forty Mile Wash. Although there may be some mixing of groundwater across Sebastian boundaries, hydrologic and hydrochemical data indicate that they form relatively distinct groundwater flow systems (DOE, 1988).

The potentiometric surface for the SZ in the immediate vicinity of Yucca Mountain indicates large variability in the magnitude of the hydraulic gradient (Luckey et al., 1996) (see Figure 6.8-2). Water-level measurements show a very small hydraulic gradient to the southeast of the potential repository with a magnitude of 0.0001 to 0.0003. A moderate hydraulic gradient is located immediately to the west of the repository as shown by a west to east decrease in hydraulic head of about 45 m. A large hydraulic gradient to the north of the potential repository might correspond to a change of nearly 300 m in water table elevation, indicating a hydraulic gradient possibly as large as 0.15 over a distance of less than two kilometers. The vertical hydraulic gradient in borehole UE-25 p#1 is upward from underlying Paleozoic age carbonate rocks to the volcanic aquifer, which are separated by an intervening aquitard. Temperature data also indicate possible upwelling of groundwater flow in some areas near the Yucca Mountain site (Sass et al., 1988).

Numerous conceptual models have been proposed to explain the observed potentiometric surface of the SZ near Yucca Mountain (Luckey et al., 1996). Most of these conceptual models have focused on possible causes for the large hydraulic gradient to the north of the potential repository. It has been pointed out that areas with large hydraulic gradients occur elsewhere in the region (Fridrich et al., 1994) and that this feature at Yucca Mountain appears to have been stable over geologic time. The implications of the large hydraulic gradient for performance of the potential repository have not been fully evaluated, but limited assessment of alternative conceptual models (e.g., whether groundwater drains from the tuff aquifer into the carbonate aquifer near the large hydraulic gradient) indicates that repository performance is not very sensitive to alternative conceptualizations (Wilson, et al., 1994).

Flow surveys in numerous wells within volcanic rocks of the SZ near Yucca Mountain indicate that major zones of water production are located in relatively discrete segments of boreholes (Geldon, 1993; Luckey et al., 1996). Hydraulic testing of volcanic rocks using single-borehole tests shows values of hydraulic conductivity spanning several orders of magnitude, depending on the stratigraphic interval tested and on the presence of transmissive fractures (Luckey et al., 1996). Multi-well hydraulic testing at the C-wells indicates much higher estimates of hydraulic conductivity (by approximately a factor of 100) relative to single-well tests for the same borehole intervals (Geldon, 1996).

Preliminary results from tracer tests at the C-wells lend support to existing conceptual models of solute transport in the SZ (Reimus and Turin, 1997). Flow and transport apparently occurs through a few discrete fractures or fracture zones at the scale of these tests. Analysis of tracer test data indicate that matrix diffusion of solute does occur and that a reactive tracer sorbs in the matrix and on fracture surfaces.

6.8.4 Issues Related to SZ Flow and Transport

A prioritized list of key technical issues related to groundwater flow and transport in the SZ was developed in a workshop for the purpose of guiding TSPA-VA analyses (M&O, 1997). These issues were prioritized on the basis of specific criteria linked to potential impact to repository performance. Workshop participants included representatives from Yucca Mountain site characterization, process-level modeling, and TSPA modeling activities. The higher priority issues identified in this process are shown in Table 6.8-1. These issues were, in turn, used to develop a set of abstraction/testing plans for the purpose of addressing these issues in abstracted models for use in TSPA-VA.

Most of these issues relate to the appropriate simulation of SZ flow and transport in numerical modeling that forms the basis of TSPA-VA abstractions. In addition, the important underlying issue in many cases is the range of uncertainty in quantifying the individual parameter/process in question. In some cases, the relative significance of the particular issue is being assessed in the abstraction/testing study plans.

The base case used in TSPA analyses for flow and transport in the SZ includes features, events and processes that are likely, have a high certainty of influencing repository performance, and/or that are prescribed by anticipated regulations. Some alternative scenarios will be evaluated using scoping calculations.

The base case scenario includes: (1) mixing of radionuclides in groundwater of the SZ at the water table, (2) advective and dispersive transport through fractured and porous media under ambient SZ flow conditions, and (3) withdrawal of contaminated groundwater in a production well for delivery to the biosphere. The location of the water well is at a distance of 5 km to 30 km from the potential repository, as defined by YMP interim requirements in anticipation of regulatory guidance. The base-case scenario also includes consideration of modified groundwater flow conditions resulting from climatic changes.

Alternative scenarios not contained in the base case include other potential methods of radionuclide release from the SZ to the biosphere, alterations to the SZ flow system due to the presence of the repository, and alterations of the SZ flow system from natural disruptive events. Natural outfalls of the SZ flow system, which form an alternative interface with the biosphere, are springs and playas. The potential repository may induce significant reversible changes in the SZ flow system from repository heat or cause durable changes in the medium of the SZ due to coupled thermal/chemical processes. Seismicity would constitute a natural disruptive event if it alters the SZ flow system.

Under existing climatic conditions, springs that could potentially discharge groundwater from the Yucca Mountain site are well beyond 30 km downgradient. Groundwater from Yucca Mountain may discharge at springs in Death Valley or may be primarily discharged by evapotranspiration at Franklin Lake Playa (Czarnecki and Waddell, 1984; Czarnecki, 1990; D'Agnese et al, 1997). Spring discharge of radionuclides would be directly available for movement into the biosphere. Evaporative concentration of radionuclides in the playa environment could result in dispersal by wind of contaminated sediments and plant debris. Under pluvial climatic conditions, spring discharge of contaminated groundwater may occur much closer to Yucca Mountain along the lower reaches of Forty Mile Wash and along the Amargosa River (Paces, 1995). The approximate concentrations of radionuclides at different potential spring discharge locations can be calculated based on extrapolation of detailed SZ transport modeling results for the base case. Any estimate of the transfer of radionuclides from playas to the biosphere would be extremely uncertain, although rough calculations of the associated buildup of radionuclide inventory at the playa would be possible.

Alterations to the SZ flow system due to the potential repository and to disruptive events will not be directly assessed in TSPA-VA analyses. These alterations are judged to be potentially significant, but highly uncertain and are not explicitly considered as alternative scenarios on this basis. Preliminary simulations suggest that the thermal plume generated by the repository in the SZ may be of significant magnitude and duration (Ho et al., 1996), but the durable changes in permeability within the SZ associated with mineral dissolution and precipitation are speculative. Several studies have concluded that changes to the SZ flow system in response to seismicity and volcanism would be relatively minor (NRC, 1992; Carrigan et al., 1990; Gauthier et al., 1996).

6.8.5 Abstraction Approach and Assumptions

The anticipated form of the abstraction of SZ flow and transport for incorporation in TSPA-VA calculations is numerical convolution of transport in the UZ with transport in the SZ. This method of abstraction permits a numerically efficient translation of the radionuclide mass flux history (as simulated by the UZ transport model) into a simulated radionuclide concentration history at a location (or locations) downgradient of the potential repository. This relatively simple transfer function, however, is based on a detailed 3-D flow and transport simulation incorporating a high-resolution model domain and relevant processes.

The strategy for using this method includes the following components. Multiple Monte Carlo SZ flow and transport simulations which encompass the range of conceptual model and parameter uncertainty are performed using the 3-D SZ model. Radionuclide concentration breakthrough curves are derived for each simulation using a hypothetical, constant, unit radionuclide mass flux at the water table below the potential repository. Concentration breakthrough curves are calculated at particular locations (e.g., points of highest concentration at 5 km, 20 km, and 30 km) and for multiple radionuclides. The results of the flow and transport simulations are performed prior to the main TSPA calculations and stored as a "library" of responses. The final component of the methodology is a numerical integration computer code that is called by the RIP program to translate the simulated radionuclide mass flux history from the UZ transport calculation into the radionuclide concentration history for the specified locations in the SZ. This numerical-convolution translation is based on the concentration breakthrough response from a single realization chosen from the "library" of responses.

The primary tool for conducting SZ flow and transport simulations will be the SZ site-scale flow model being developed at the US Geological Survey (Czarnecki et al., 1997) and the accompanying SZ transport modeling analyses at Los Alamos National Laboratory (Zyvoloski et al., 1997). These simulations are being conducted using the FEHM computer code (Zyvoloski et al., 1996). In addition, detailed sub-site-scale SZ flow and transport modeling will be used to evaluate the influence of discrete flow channelization features and to analyze dilution at pumping wells.

The radionuclide concentration breakthrough curves will be determined for locations with the highest radionuclide concentration for a given distance downgradient (i.e., the center of the simulated contaminant plume) assuming a constant unit mass flux source. The breakthrough curves for each SZ flow and transport simulation will be included in the "library" of simulations. Each entry in the "library" will be associated with a vector of parameter values used in the parent SZ flow and transport simulation. There will be two or more simulations for each set of flow and transport parameters, one for ambient, present-day flow conditions and one or more for wetter, pluvial climatic conditions. An entry from the "library" will be chosen at random for each realization of the RIP program. The response in the SZ will be switched back and forth from ambient to the corresponding climate-change conditions entry, in synchronization with the simulated climatic conditions in the other components of the TSPA simulation.

The convolution integral method is a relatively straightforward method of translating a transient input function into a transient output function based on the response of the system to a unit step function at the input boundary. The method is implemented using numerical integration over the time of interest. The major assumptions inherent in the method, as applied here, are that steady-state flow conditions exist in the SZ and that transport processes are linear in the SZ. Changes in the SZ flow system associated with climate change will be approximated as a "jump" from one steady-state flow solution to another steady-state flow solution. Estimates of the transient response of the SZ flow system to climate changes are not presently available and the steady-state-to-steady-state approximation is being used in other components of TSPA calculations. Because of the abrupt simulated changes to the system inherent in this approximation, the results will be conservative from the perspective of repository performance. Verification of the convolution integral method is accomplished by comparing the simulation results of a SZ flow and transport model in which the transient radionuclide mass flux source is explicitly specified to the results of the convolution integral method in which the same transient mass flux source is applied. This verification procedure checks both the implementation of the numerical integration and the assumption of the linearity of transport processes in the SZ.

Another form of abstraction will be used for estimating the dilution of radionuclide concentrations at groundwater withdrawal wells. This dilution factor will simply be used to divide the simulated radionuclide concentration at points of interest and will be treated as an additional uncertain parameter. The basis for the well withdrawal dilution factor is a set of numerical simulations of SZ flow and transport from a pumping well located within the simulated radionuclide plume. This dilution factor is the final concentration in the well relative to the maximum pre-pumping concentration at that location. The calculated dilution factor is primarily a function of the well withdrawal rate and the width of the simulated contaminant plume. Higher well withdrawal rates and longer well-screen intervals lead to a greater dilution factor. Greater dilution from pumping also occurs nearer the repository where the simulated plume is more compact, relative to the dilution expected at greater travel distances where the plume is broader. The well dilution factor is calculated assuming steady-state conditions for flow and transport to the withdrawal well, which are expected to occur relatively rapidly for large-capacity wells.

6.8.6 Base Case and Sensitivity Cases

For TSPA-VA, flow and transport in the SZ will be based on the USGS 3-D flow model (Czarnecki et al., 1997) and the LANL 3-D transport model (Zyvoloski et al., 1997), as abstracted by the convolution integral method. Some parameter variations will be incorporated in the 3-D calculations, including different permeabilities, dispersivities (longitudinal and transverse), sorption coefficients, etc. The base case will represent the base-case scenario discussed in Section 6.8.4, above.

Climate change will be considered in the base case. We anticipate that saturated-zone flow and transport will be calculated for ambient (present), long-term average, and pluvial climates. Convolution integrals will be developed for each of these climates and, during a given realization, when a climate change is to occur, the calculation will abruptly change from one flow and transport state to another.

For TSPA-VA, sensitivity analyses will be conducted to look at alternative conceptual models of the SZ. A preliminary listing of possible sensitivity analyses follows.

- Examine the effect of channelization of flow in the SZ, i.e., flow disequilibrium between matrix and fractures extends across many grid cells. Channelized flow is a characteristic of fractured-rock aquifers, yet its effect on transport over long distances and times is not known. Channelization could increase effective flow velocity and reduce dispersivity, matrix diffusion, and retardation (reduce effective porosity and sorption coefficients).
- Examine the effects of repository heating and chemical changes on SZ flow and transport, including convective flow in the SZ and the chemical plume that will accompany transporting radionuclides.
- Examine the impact of colloidal transport of strongly sorbing radionuclides, in particular plutonium, on repository performance.
- Determine how well the methodology planned for the TSPA calculations (the convolution integral method and the steady-state-to-steady-state jump for climate change) match transient calculations.
- Examine alternative conceptual models of flow in the SZ; e.g., whether the large-hydraulic gradient to the northwest is actually the water table or perched water, whether there is a groundwater divide through the repository footprint, etc.
- Examine different hydraulic properties of faults; e.g., whether they might be more or less permeable.
- Investigate the possibility of vertical flow between aquifers in the SZ, and its possible effect on mixing depth,. A positive head has been measured between the underlying carbonate aquifers and the tuff aquifer at UE25p#1; temperature measurements suggest upwelling at faults.

- Investigate UZ flow and transport coupling with the SZ and whether radionuclides could be delayed at this interface, whether dilution in the SZ water could be limited, etc.
- Investigate different well-withdrawal scenarios; e.g., pumping depths.
- Investigate any inconsistencies between the site-scale and regional-scale flow models and determine their potential impact on the TSPA-VA.

6.8.7 References

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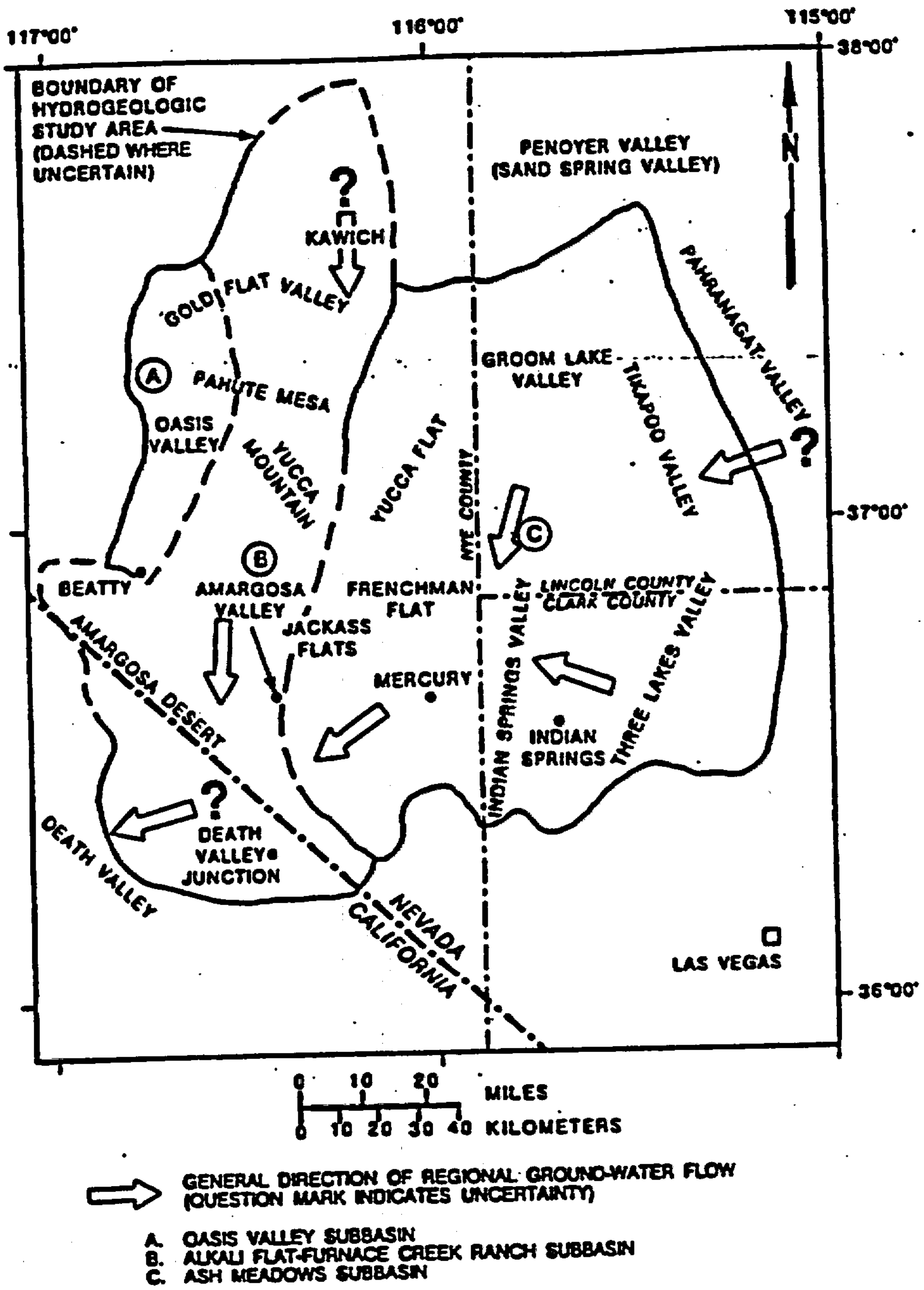

Figure 6.8-1. Regional groundwater flow system, showing three groundwater subbasins (from DOE, 1988).

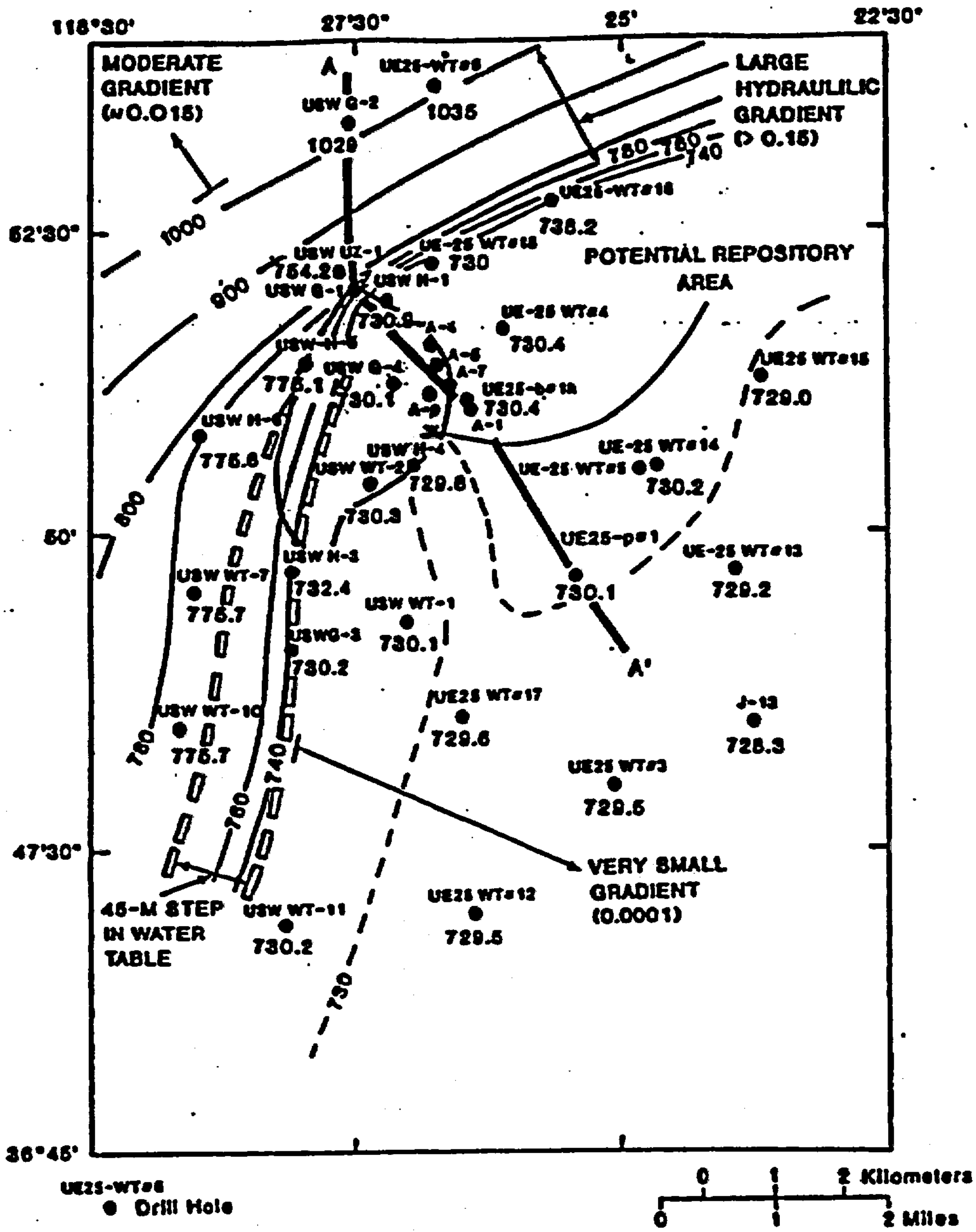

Figure 6.8-2. Potentiometric surface and water level measurements in the vicinty of Yucca Mountain (from Fridrich et al., 1994). Water levels given in meters above mean sea level.

6.9 BIOSPHERE

John H. Gauthier, Anthony J. Smith, Jeffrey J. Tappen

6.9.1 Introduction

The biosphere is the region of the planet that is occupied by living organisms. The radioactive wastes that will be placed in the repository only impacts humans or other life forms when it reaches the biosphere. The previous sections of this report discuss the transport of the radionuclides in the geosphere to the interface with the biosphere. The portion of TSPA discussed in this section, the "biosphere", addresses the transport of radionuclides once they have been introduced, by feasible mechanisms, into this region of the Earth. The biosphere has been defined by National Academy of Sciences (NAS, 1995) as, *"The region of the earth in which environmental pathways for the transfer of radionuclides to living organisms are located and by which radionuclides in air, ground water, and soil can reach humans to be inhaled, ingested, or absorbed through the skin. Humans can also be exposed to direct irradiation from radionuclides in the environment."*

For the proposed repository at Yucca Mountain, interest has been focused on the human population that could receive the highest dose as a result of radionuclides released from the potential repository. In the absence of a Federal Regulation for the high level waste repository, the metric that is being employed to quantify the capability of the mountain to safely isolate the radioactive waste is the ionizing radiation dose to a reference person in the area. This dose requirement has been defined by DOE (DOE, 1997) as *"The expected annual dose to an average individual in a critical group living 20 kilometers (km) from the repository shall not exceed 25 mrem from all pathways and all radionuclides during the first 10,000 years after closure."* A post-10,000 year qualitative goal of not exceeding this does level was also defined by DOE.

Radionuclides from a potential repository at Yucca Mountain would travel first through the geosphere, to the biosphere, by different "pathways." To date several possible pathways have been subjected to study. The most studied pathway to date has been the one expected to take place under anticipated future conditions. This pathway is the mobilization and transport of the radionuclides by the natural flow of ground water. This water is then assumed to be used, as it is at present, to support a critical group, with drinking and irrigation water. Another possible pathway is via volcanic activity, which potentially could disperse radionuclides in the atmosphere where they can then be inhaled, as well as spread over the region in a carpet of volcanic ash which can later be farmed on. An additional pathway is as a result of inadvertent human intrusion, where exhumed radionuclides can irradiate drilling crews or miners, and then be left on the surface to be dispersed by the forces of nature and waste can be directly transported into the saturated zone by the drilling. A fourth pathway, for radionuclides that are in the gaseous state, is diffusion through rock and soil, into the atmosphere, where they can be inhaled by humans or incorporated into the food chain by plants. Other pathways may also be postulated.

Previous TSPAs have indicated that pathways involving unlikely or rare events, specifically farming on ground contaminated by wastes from drilling through the repository, lead to the highest doses. However, the groundwater pathway occurs without any external event or process other than precipitation and is judged to be the primary route for radioactive releases and consequences. This is the pathway that will be addressed by TSPA-VA biosphere-modeling efforts.

As with any natural system, the analysis of the biosphere holds inherent variabilities and uncertainties. One of the obvious variabilities is that all humans do not have the same habits, do not grow and eat the same things, do not drink the same amount of water, nor do they spend the same time outdoors. An obvious uncertainty is the state of human society, technology, and habits at some point in the distant future when the radionuclides are expected to reach the biosphere. Although the characteristics of future human activities cannot be accurately predicted, an attempt is made to address the problem by identifying the critical group (the group of maximally exposed individuals) by (1) basing parameters on survey data of existing inhabitants of the area around Yucca Mountain, (2) using techniques and metrics that are acceptable to the international community of experts studying the biosphere for radioactive waste disposal, and (3) performing probabilistic calculations wherein selected parameters are sampled from probability distributions.

6.9.2 Previous TSPA Modeling

The first (and most comprehensive in terms of pathways), examination to date of the Yucca Mountain biosphere in a TSPA was undertaken for TSPA-91 (Eslinger, et al., 1993). Scenarios were developed to investigate both waterborne and surface contamination from both an undisturbed repository and a disrupted repository. For the undisturbed repository, scenarios were as follows: (1) drinking-water only, and (2) farm exposure, including drinking water, irrigation, all foodstuffs, and direct ionizing radiation exposure. For the disrupted repository, the scenarios were as follows, (1) exposure of a driller to inhaled contaminated dust and exposure to external contamination, (2) garden exposure, involving living and gardening on soil contaminated by the remnants of exploratory drilling, and (3) external only, involving only residence on land contaminated by previous drilling through the repository. Parameters in these analyses were all deterministic i.e., specified exactly (i.e., the calculations were not probabilistic), except that exposures were calculated for different repository lifetimes. Most simulations covered only 10,000 yr, although some went out to 1,000,000 yr. Results of analyses showed that the disrupted-repository analyses generated the largest doses, especially the garden-exposure scenario.

For TSPA-93 (Andrews, et al., 1994; Wilson, et al., 1993), emphasis was primarily on the dose incurred from drinking contaminated water. Andrews, et al. (1994) also considered the effect of crop irrigation. The drinking well was assumed to be screened in a 50-m interval and placed in the contaminant plume.

For TSPA-95 (M&O, 1995), only the drinking-water pathway was considered. Since then, the contribution of drinking-water dose to the total dose from all potential sources has been investigated. It has been determined that in some cases, especially those involving persons ingesting mostly food produced using contaminated water (where the food concentrates radionuclides), the total dose could be an order of magnitude or greater than the drinking-water only dose; i.e., the drinking-water dose could be a small contributor to the total dose. The results of these analyses, which are consistent with those reported by the Electric Power Research Institute (EPRI) (Kessler, et al., 1996), demonstrated the necessity for a more detailed biosphere model for TSPA-VA.

TSPA modeling of a Yucca Mountain repository by other groups outside of the Yucca Mountain Project have also investigated the biosphere. In particular, EPRI (Smith, et al., 1996) developed a comprehensive list of features, events, and processes (FEPs) affecting radionuclide transport from a repository at Yucca Mountain and an interaction matrix relating them. Also produced were a definition of the "critical group" for their assessment of the Yucca Mountain environs, and a list of parameter values, including uncertainty ranges, for dose calculations. In the dose calculations (Kessler, et al., 1996), a maximally exposed individual, a single farm, a small population, and a large population were considered. Pathways scenarios included drinking water and all pathways exposures. Water was assumed to come from a well in the plume of the contaminant flow from the repository. The well water was used for irrigation and livestock watering. The calculations were probabilistic and based on estimates of existing agriculture in Amargosa Valley, approximately 25 km downstream from Yucca Mountain (although the modeled distance from Yucca Mountain varied for different scenarios). Results of this study (and TSPA-95) showed that the radionuclides and pathways of importance to dose varied over time. For example, the dose from Se-79 via ingestion of cow liver was predicted to be the major contributor to dose in a time window around 200,000 yr for the scenario involving a "conservative individual" located 5 km from Yucca Mountain. Before this time window, Tc-99 was predicted to dominate the dose, while at later times U-233 dominated.

6.9.3 General Description

Yucca Mountain lies in an arid, sparsely populated region of the southern Great Basin in southern Nevada. Evaluation of water-flow and wind patterns suggests that any contamination from a repository at Yucca Mountain would likely hydraulically spread south (Czarnecki, 1997; D'Agnese, 1997) and atmospherically to the south east (CRWMS M&O, 1996) respectively. Vegetation is primarily desert scrub and grasses. The mean annual precipitation in these areas is between 100 and 150 mm/yr and the mean annual temperature is about 18 degrees Celsius. The closest settlement is at Lathrop Wells, approximately 20 km to the south on Highway 95. The closest area where agriculture is practiced is the Amargosa Valley, approximately 30 km to the south (Figure 6.9-1).

A survey of the Amargosa Valley and neighboring areas is being undertaken by the YMP to define demographics. A pilot study of the region was undertaken to facilitate defining the more comprehensive survey. This unreported pilot study of the Amargosa Valley indicated that the population numbers around a thousand in about 280 to 400 households. Some type of locally produced food was consumed in 76% of the households in the previous 12 months (Survey, 1997). A focus group of 13 Amargosa Valley residents indicates that water is predominantly acquired from wells for household uses, agriculture, horticulture, and animal husbandry.

Scientific evidence indicates the biosphere has changed over similar time scales of interest to TSPA. Ignoring changes in human habits, societies, and technology (which are generally considered to be unpredictable over long periods of time), we note that climate and vegetation have been different in the past and can be anticipated to be different in the future when compared to present conditions. The climate during the last glacial period (approximately 20,000 yr Before Present) was colder and wetter than present, with precipitation having been approximately twice to three times the present value and temperature having been approximately 5 degrees colder. There were more instances of surface water in the form of springs and marshes than at present (i.e., only Ash Meadows). These outflows were at the southern end of Crater Flat, at Fortymile Wash, and at the Nevada/California state line. Fauna included large mammals, such as mammoths and camels, along with the flora needed to support them.

6.9.4 Important Issues Related to the Biosphere

A workshop devoted to determining important issues related to the biosphere, and courses of action to address these issues, was held in Las Vegas, NV, on 2-3 June 1997. A list of potential issues was produced by the organizers and supplemented by the workshop participants. The list was prioritized according to three criteria: (1) the effect on individual dose; (2) the effect on population dose; and (3) the range or uncertainty that the issue implied for determining Biosphere Dose Conversion Factors (BDCFs--see Section 6.9.5). Issues that were prioritized highest were to be addressed further if possible, either by abstraction into a model for TSPA-VA or by investigation as the subject of a sensitivity study. (Because of the short period of time between the workshop and the date when biosphere results would be needed for inclusion in TSPA-VA, the fall of 1997, it was recognized that not all issues would be addressed. However, it is expected that all significant issues will be considered for the next phase of the TSPA process, TSPA-LA) Table 6.9-1 lists the important issues determined at the workshop.

The first category, "Critical Group," concerns how to represent the human or humans that would be the basis of a dose calculation. "Extrapolation of habits to future" concerns how the human inhabitants of the region will behave in the future--a speculative endeavor. "Habits of critical group" concerns how the present inhabitants of the region behave, in particular what are the behaviors that would result in the greatest doses. "Location of critical group" concerns how far from a repository would the impacted humans live, and therefore how dilute the contaminant stream would be.

The second category, "Climate," concerns how to represent the future environment in a dose calculation. "Effects of climate change on biosphere pathways" concerns physical changes to the environment and the consequences; e.g., increased rainfall causing reductions in dust and irrigation. "Effects of climate change on critical group" concerns demographic changes in the human population receiving the potentially greatest dose; e.g., increased rainfall causing greater consumption of locally produced foods. "Soil build-up" concerns the accumulation of radionuclides in soil over time because of continuing irrigation, rain water wash out, and/or evapotranspiration.

The third category, "Pathway Variability," concerns factors affecting movement of radionuclides through the environment to the critical group. "Location and definition of Bio-Geo interface" concerns where and how radionuclides leave the geosphere to become accessible to the biosphere. "Range of uncertainties and variability in parameters and pathways for critical group" concerns how well the pathways can be characterized and how uncertainties and variabilities can be represented; e.g., what is the range of values that should be considered for the plant-uptake parameter as these are dependent on plant species, soil type, irrigation method, fertilizer source, etc. (See Section 6.9.6). "Variation in dominant pathways with time" concerns how the major pathways of importance might change with future climates or changes in human behaviors. "Radionuclides of importance" concerns limiting, to a manageable set, the radionuclides that must be considered in a defensible dose calculation. "Volcanism" concerns what factors must be considered to look at the scenario of radionuclides released by volcanic events; e.g., inhalation of ash or farming on ash-covered soil. "Which radionuclides and how transferred in disruptive scenarios" concerns the set of radionuclides that must be considered in a defensible dose calculation for a disruptive event. "Inadvertent intrusion" concerns how to calculate the dose received by persons exhuming radioactive waste from a repository; e.g., the dose to exploratory drillers that inadvertently penetrate a waste package.

Three analysis plans are being developed to address as many important issues as possible and as practical in the time available before TSPA-VA. Briefly, the analysis plans are as follows. (1) "Provide appropriate BDCFs to TSPA." This analysis will define a reference person and a reasonable set of pathways, and calculate the dose ultimately received by the reference person from a unit concentration of a given radionuclide at the geosphere/biosphere interface. Survey data will be used to define the characteristics of the reference person and associated pathways. Alternative scenarios will be developed. Calculations will be probabilistic. (2) "Determine the radionuclides that are significant contributors to dose." Based on a sensitivity study and previous TSPAs, a list of radionuclides will be developed for use in calculating BDCFs. (3) "Provide consistency between radionuclide concentrations in the saturated zone and biosphere scenarios." The geosphere/biosphere interface will be defined in order to make adjustments to the concentrations of radionuclides in the geosphere at the point of contact with the biosphere; e.g., well pumping will be investigated as a source of dilution.

6.9.5 Abstraction Approach and Assumptions

The biosphere will be abstracted in TSPA-VA by using the concept of Biosphere Dose Conversion Factors (BDCFs). A BDCF is a multiplier that converts a radionuclide concentration at the geosphere/biosphere interface into a dose to a human for all pathways considered. The units are in terms of annual dose (more specifically the total effective dose equivalent) per unit concentration, e.g., rem/mg/l, Sv/Bq/m^3, etc. BDCFs are radionuclide dependent, scenario (which pathways are considered) dependent, climate dependent, etc. The BDCFs to be defined for TSPA will consider the critical group and all the appropriate pathways for that group and scenario. Thus there will be a single BDCF for each radionuclide for each scenario.

Implicit in the use of BDCFs is that dose is a linear function of concentration at the geosphere/biosphere interface. This assumption is generally valid at the anticipated low levels of contamination that will be acceptable. BDCFs should not be confused with Dose Conversion Factors (DCFs). DCFs are the multipliers that convert an amount of radionuclides ingested or inhaled to an estimate of dose. The units are in terms of dose per activity, e.g., rem/Ci, Sv/Bq, etc. As with BDCFs, implicit in DCFs is that the radionuclide intake and external radiation exposure is for a year, but the dose is that accrued by the individual over a 50 yr period (i.e., the dose is committed). In calculating the BDCF for each element, the biosphere model estimates the quantity of each radionuclide taken into the body (by inhalation and ingestion) and the DCF converts these amounts to dose in the usual manner.

BDCFs contain many uncertainties, receptor variability, pathways considered, uptake rates, compartment exchange rates, etc. For TSPA-VA, BDCFs will be calculated in a probabilistic manner and will have some measure of uncertainty, e.g., standard deviation or error bars. When used in the TSPA-VA calculations of consequences, each isotope BDCF will be sampled from the parent distribution.

6.9.6 Base Case and Sensitivity Cases

The base case for TSPA-VA will consist of the reference adult person living 20 km from Yucca Mountain. The reference person will be defined using a survey of the existing population. The person will eat locally produced food at proportions similar to those determined by survey. The person will spend time outdoors an amount similar to that determined by survey, and have other habits similar to those determined by survey. Climate change will be factored in if it is determined that it will materially change the BDCFs. Changes in the reference person because of potential changes in demographics over time will not be considered.

Water for drinking and for food production will be from a well intercepting the highest concentration point (at 20 km) of a plume of contaminated groundwater from Yucca Mountain. Concentration will be reduced at the well head because of mixing with uncontaminated water during pumping; the reduction will be determined in an ancillary calculation and will be dependent on pumping rate (see Section 6.8.5).

Only pathways involving contaminated groundwater pumped from a well at 20 km from Yucca Mountain will be considered in the base case.

Radiation dose will be calculated (using BDCFs) all significant radionuclides and all significant pathways. The radionuclides (12) presently being considered for the detailed biosphere study are as follows: C-14, Cl-36, Se-79, Tc-99, I-129, Th-229, Np-237, Ac-227, Pa-231, Pb-210, Pu-239, and Pu-242. These radionuclides were estimated to be the major contributors to dose, using the present TSPA predictive models (not the TSPA-VA models) and published tables of generic *screening factors* (NCRP Report No. 123, 1996) and were estimated to account for about 99.9% of the radiation dose at any time of concern. The contribution arising from the "other" radionuclides, that are anticipated to account for about one percent of the total dose, will be generated for the TSPA-VA calculations by using generic (i.e., not site specific for the Yucca Mountain region) BDCFs for the critical group. Because of the small dose contribution expected from these radioisotopes, the approximate nature of the BDCFs will not impact the TSPA-VA findings. The dose from each radionuclide will be calculated at multiple time steps in the TSPA calculation (at each time step, if appropriate) in order to determine the magnitude and time of the peak total dose and individual contribution to the total. The peak doses from multiple simulations (realizations), which will include the sampling of different BDCFs, will be collected in a complementary cumulative distribution function for presentation.

BDCFs for the base case will be determined by probabilistic calculations, i.e., parameters will be sampled from parent distributions and the final result, a BDCF for a given radionuclide will be in the form of an anticipated statistical distribution. Parameters that are presently being considered for probabilistic definition include plant uptakes, uptake of plants by animals, irrigation rates, annual precipitation level, human consumption rates, fraction of locally produced foodstuffs consumed, time spent outdoors, amount of dust inhaled, soil-buildup factors, etc. Parameter values will be taken from authoritative sources (e.g., Coughtrey, 1990, and IAEA, 1994.) DCFs for the calculation will not be sampled; deterministic values will be taken from a published source Federal Guidance Reports Nos. 11 & 12. If sensitivity of dose to geosphere variability is being marked by biosphere variability, a deterministic biosphere calculation will be used to judge dose sensitivity to the geosphere.

Some consideration will be given to other areas of interest. At present these ancillary evaluations will be based, to the extent possible, on the above mentioned biosphere effort. First an assessment will be made of the probable changes in BDCFs that would result in changes in the current mandated 20 km distance for the critical group. In particular, interest has been shown in the dose estimates at 5 and 30 km distance. As seen previously there is a great effect in the concentration and distance to release of each radionuclide with distance. However the effect of distance on the biosphere BDCFs are thought at present to be subtle and swamped in the current uncertainties of the many required parameters. This distance scaling will be investigated as a sensitivity study on location of the critical group for VA as a sensitivity study on the location of the critical group.

It is planned that alternative release mechanisms from the repository will be evaluated. The biosphere workshop identified such releases as of relative low priority in the VA time horizon. (Note these and other issues will be addressed in much more detail for LA.) Resources are deployed on those issues considered important and there is no plan for a detailed biosphere modeling of these releases to support VA. The releases are those arising from volcanism and inadvertent intrusion (drilling activities). Estimates of BDCFs will be derived for these release mechanism using more generic approaches, if for no other reason that they contain many more radionuclides (i.e., the complete inventory). The effect of climate change on the biosphere portion of the dose calculation will be estimated using existing tools that allow for variable irrigation rates, dust generation, soil build-up/wash-out.

6.9.7 References

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Table 6.9-1. Issues Important to the Biosphere.

Category	Issue
Critical Group	1.3 Extrapolation of habits to future 1.2 Habits of critical group 1.4 Location of critical group
Climate	2.10 Effects of climate change on Biosphere pathways 1.5 Effects of climate change on critical group 2.1 Soil build-up
Pathway Variability	3.7 Location and definition of Bio-Geo interface 1.7 Range of uncertainties and variability in parameters and pathways for critical group 1.9 Variation in dominant pathways with time 2.6 Radionuclides of importance 3.4 Volcanism 3.5 Inadvertent Intrusion

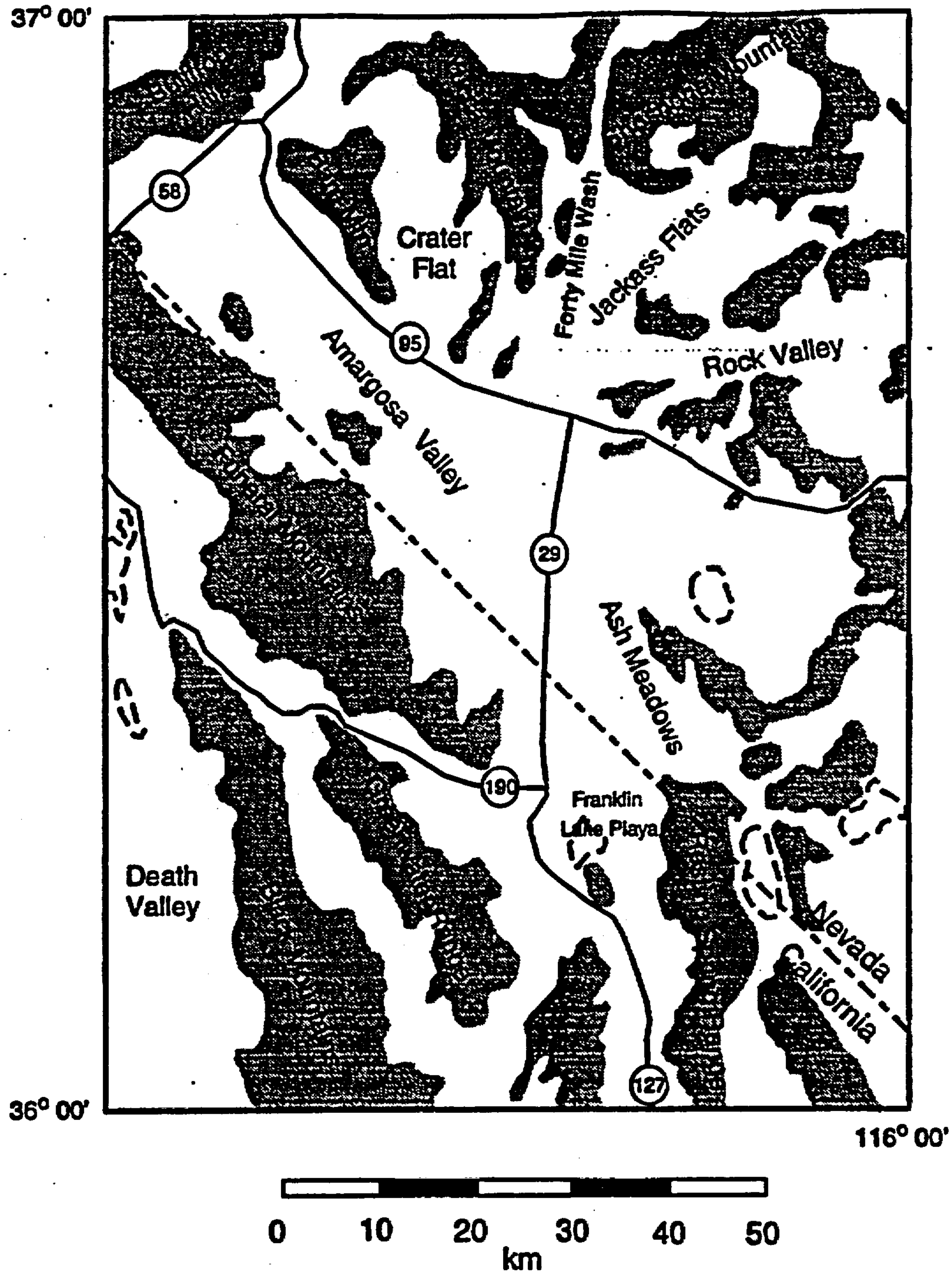

Figure 6.9-1. Yucca Mountain Vicinity with Some Locations Important to Biosphere Investigation

6.10 DISRUPTIVE EVENTS

Ralston W. Barnard

6.10.1 Introduction

Disruptive events to be considered in TSPA-VA include igneous activity, seismicity/tectonism, nuclear criticality, and human intrusion. Disruptions to the repository and surroundings can occur from both direct and indirect effects of volcanism and/or earthquakes, as well as inadvertent human intrusion such as drilling. Nuclear criticality could occur when fissile materials in the radioactive waste combine with other specific environmental conditions required for criticality.

Although analyses of disruptive events are not included in the base case performance analyses, they are important tests of the robustness of the repository design and of the isolation assumed to be provided by the natural site features. Disruptive events are reported in terms of the sensitivity of repository total-system performance to the disruptions.

The analyses of disruptive scenarios for TSPA-VA attempt to exhaustively identify the features, events, and processes (FEPs) in the several scenario classes. The number of scenarios that can be analyzed in a TSPA is limited, however. The scenarios intended for inclusion in TSPA-VA fall into the following categories: (1) those that were included in prior TSPA analyses and were criticized in some regard, (2) those that are judged to be of high consequence to repository performance, (3) those that have a frequency of occurrence such that they are likely to occur over the repository lifetime, (4) those that are of high probability (but possibly low consequence), and (5) those that may not have a significant impact on performance impact, but are of high public concern.

Some disturbed conditions are of concern because of regulations. For example, nuclear criticality is a concern because it is one of the subsystem requirements imposed by the NRC (as given in 10 CFR 60.131(h)). That requirement states "... that a nuclear criticality accident is not possible unless at least two unlikely, independent, and concurrent or sequential changes have occurred in the conditions essential to nuclear criticality safety."

6.10.2 Treatment in Previous TSPAs

Igneous- and human-intrusion disturbances were included in both TSPA-1991 (Barnard et al., 1992) and TSPA-1993 (Wilson et al., 1994). Seismic effects have been calculated in 1995 as a sensitivity study using the TSPA-1993 as the starting point. Nuclear criticality has not been treated in a TSPA analysis before, although some calculations of the PA consequences have recently been done as part of the Disposal Criticality Methodology report (CRWMS M&O, 1997a).

6.10.2.1 Igneous Activity

In TSPA-1991, direct releases at the surface from magmatic entrainment of waste were investigated. Stochastic analyses were performed; because the probability of occurrence of igneous activity is so low (a range of 10^{-7} to 10^{-6} per year was used in that analysis – Crowe, 1991), consequences of volcanism were calculated separately and combined with the probability to give a final measure of impact on repository performance. The model considered the intrusive dike orientation, length, and width to be random parameters. Probability distributions for these parameters were developed from data obtained from the volcanic cones adjacent to Yucca Mountain (Crowe et al., 1983; Valentine et al., 1992). Models for waste entrainment were developed from observations of wall-rock entrainment in the Crater Flat area. Results showed that direct releases contributed a risk (consequence times probability) at least four orders of magnitude lower than the then-applicable EPA standard given in 40 CFR Part 191. A separate contribution to TSPA-1991 (Eslinger et al., 1993) used a more conservative basis and showed similar results, suggesting that volcanism was not likely to be an important contributor to releases from a Yucca Mountain repository.

In TSPA-1993, the effects of a magmatic intrusion to accelerate waste degradation were modeled. The increased temperature and the presence of aggressive chemicals in the vicinity of a dike intrusion were modeled as causing accelerated corrosion of waste packages and waste form. The exposed waste was then assumed to be available to be transported by groundwater flow. Results showed that the incremental increase in groundwater-borne doses was about 10^{-8} of the EPA sum in 10,000 years from this igneous disturbance.

6.10.2.2 Human Intrusion

Both TSPA-1991 and TSPA-1993 investigated direct surface releases from drilling into the repository. In the former analysis, transport of contaminants in drilling fluids from both direct hits and "near misses" (contaminated rock adjacent to a degraded waste package) were modeled. In TSPA-1993, only direct hits were studied. Additionally, TSPA-1991 considered releases arising from depositing waste at the bottom of a borehole that reached the saturated zone. In all cases, the models were predicated on the probability of a drill bit intercepting a waste package and breaking it open. This probability was based on geometric arguments, that were dependent on the size and spacing of the waste packages, and the number of boreholes drilled into the repository over a given time period. Using EPA guidance for the number of boreholes likely to be drilled into the repository (EPA, 1985), there is about an 11% chance of one intersection in 10,000 years. For both small waste packages (the SCP design) or large ones (approximately the current design) the risks due to surface releases are about two orders of magnitude below the EPA standards. The saturated-zone releases were analyzed in TSPA-1991, and assumed that the entire contents of one SCP-size waste package (approximately 2.1 metric tonnes) were deposited in the saturated zone. It was further assumed that the radionuclides were immediately mobilized and transported by the groundwater. The results showed that the risk from this disturbance was over two orders of magnitude below the then effective EPA standard. Similarly, Eslinger et. al (1993) found little contribution to releases from human intrusion.

6.10.2.3 Seismic Activity

Seismic disturbances (rockfall, fault displacement, alteration of groundwater flow patterns, and water-table change) have been modeled using the TSPA-1993 analyses as the starting point (Gauthier et al., 1996). These calculations were undertaken after TSPA-1993 and are not part of that effort. The effects of rockfall in a repository drift without backfill are potentially three-fold: direct damage if large blocks fall on a waste package, increases in thermal insulation, and capillary water pathways from a covering of rock. Faulting can directly affect waste packages by changing water-flow patterns to increase corrosion rates, or by shearing otherwise mechanically degraded containers due to an increase in strain along the fault rupture; earthquakes can cause strain-induced changes in the water-table elevation. Similarly, earthquakes can redistribute the strains in fractured rock that could open or close some fractures or faults. TSPA-1993 analyses originally assumed that the repository drifts were backfilled after emplacement of the waste. The aqueous releases and doses predicted for analyses including rockfall are essentially the same as those originally calculated for TSPA-1993. One model for groundwater–waste-package interaction (the weeps model) indicates that seismically induced altered flow paths can cause an increase in doses over long periods of time (1,000,000 years, in these analyses).

The extent of water-table rise as a result of faulting has recently been reported (Carrigan et al., 1991; NRC-NAS, 1992; Arnold, in press). For a 1-meter fault displacement in the repository block (equivalent to approximately a magnitude 6.8 earthquake at Yucca Mountain) transient water-table elevation increases were predicted. The water elevation increases do not result in fracture saturation at the repository horizon. In fact, observations of water-table elevation changes arising from earthquakes outside the repository block indicate that water-table changes are of the order of only a few meters at the Yucca Mountain site (O'Brien, 1993). This work has not been incorporated into a TSPA analysis and the transmit nature of the effect makes it an unlikely contributor to performance.

6.10.2.4 Nuclear Criticality

As part of the analyses prepared by the YMP Waste-Package Design organization, sample nuclear criticality investigations have been performed. These models assumed that waste-package and waste-form degradation occurred that permitted a critical configuration to form, and that the other necessary conditions (sufficient nuclear fuel, presence of neutron moderators, absence of neutron absorbers, and favorable geometry) were obtained. As a result, the consequences of criticalities of up to 10,000 years' duration were estimated. The greatest PA consequences of such criticalities would be if they produced sufficient long-lived, mobile radionuclides that could increase the dose at the accessible environment. The preliminary findings were that increases in inventory of such radionuclides were less than 5% above the limited subset of the original inventory assumed to go critical (CRWMS, 1997a). Prompt criticality is extremely unlikely and does not warrant inclusion in a TSPA.

6.10.3 Disturbances to be Included in TSPA-VA

The frequency of occurrence for an igneous intrusion into the repository has been estimated in the Probabilistic Volcanic Hazard Analysis (PVHA) report (CRWMS, 1996a) as having a mean value of about 10^{-8}, with a maximum of 10^{-7} per year. This frequency puts volcanism into the range where the NRC considers the risk to be not insignificant. For TSPA-VA, three types of consequences will be studied: (1) direct releases to the surface from volcanic eruptions, with subsequent dispersal of radionuclides; (2) changes in the amounts of radionuclides available for transport by groundwater as the consequence of a nearby igneous intrusion; and (3) indirect effects (such as alteration of saturated-zone flow and transport) from an igneous intrusion outside the repository block.

Nuclear criticality can occur in three locations after emplacement of the waste in the repository: (1) inside a damaged waste package, (2) in the near field immediately adjacent to a damaged waste package, and (3) in the far field (either the unsaturated or saturated rock of Yucca Mountain and beyond). Almost every waste package contains sufficient fissile material to support criticality — provided the engineered criticality-suppression features are eliminated, and other conditions necessary for maintaining neutron multiplication are met. Thus, most emphasis is placed on investigating scenarios that can lead to in-package criticalities. Next in probability are near-field criticalities; lastly, critical configurations in the far field require re-concentration mechanisms that must be identified as being possible in the Yucca Mountain environment. Prompt criticality (i.e., a nuclear explosion) is so unlikely as to not be considered.

The impacts of seismic events are being considered in repository design and operations, but have not yet been thoroughly studied for their effects on post-closure repository performance. When the Probabilistic Seismic Hazard Analysis (PSHA) report becomes available, the probabilities and consequences of direct and indirect seismic events can be modeled. The disturbances to be modeled include: (1) effects resulting from seismically induced waste-package failures; seismic damage to waste packages includes rockfall and damage from ground motion and displacement; (2) effects on repository performance include increased aqueous or gaseous releases arising from an increased radionuclide source term; (3) indirect effects (such as alteration of saturated-zone flow and transport) from an earthquake located outside the repository block; and (4) effects of water-table rise on contaminant transport by groundwater.

Evaluation of the impact of human intrusion on the potential repository presents a different problem than for other disturbed scenarios. Because of our acknowledged inability to predict the state of human technology, society, or institutions in the future, we cannot even remotely hope to assign a probability to inadvertent human intrusion activities. Therefore, the National Academy of Sciences (NRC-NAS, 1995) recommended in their report: "Technical Bases for Yucca Mountain Standards" that only a condition consequence analysis for inadvertent human intrusion resulting from drilling into the repository be performed. Lacking a probability component, these results could not be included in the overall measure of risk to the public from the repository. Instead, the analyses could be used to show the degree of robustness of the natural features and the engineered systems to a stylized human intrusion event. Furthermore, the NAS report recommended that only the impacts arising from compromise of the repository engineered and natural barriers be evaluated; hazards from direct releases at the surface due to drilling would be more a function of the nature of the hazard of the waste itself than of the repository design or location. Based on this reasoning, TSPA-VA will analyze doses to the public resulting from transporting the contents of one waste package directly to the saturated zone as a consequence of drilling into the repository.

6.10.4 Important Issues

The features, events, and processes (FEPs) that form the scenarios for disturbances to be analyzed are now presented. The FEPs are organized into generalized event trees that attempt to present an exhaustive depiction of ways that failure (i.e., release of radionuclides) can occur for a given class of disturbances. Because the disturbances are treated as perturbations to the base case, their incorporation in the overall results is a three-part process. One part is the identification of the nature of the disturbance leading to releases or perturbation of the base case. Examples are transport of waste to the surface by volcanism, or increase in the repository radionuclide inventory from a nuclear criticality. Another part is the determination of whether the disturbances have any effect on the performance of the repository; thus, if a criticality creates additional fission products at the repository, but they do not increase the dose at the accessible environment, there is no significant consequence from the criticality. Finally, probabilities of occurrence are estimated for the disturbance. The combination of dose consequence and probability gives the dose risk of the disturbance.

The FEP diagrams do not necessarily reflect equally likely scenarios. In the interest of being exhaustive, some paths through the tree are shown that can be dismissed by expert review as being improbable. In some cases, detailed analyses of FEP tree branches will identify whole scenarios that can be dismissed.

6.10.4.1 Igneous Activity

The top-level FEP diagram for igneous activity is shown in Figure 6.10-1. The first branch of the diagram shows igneous intrusions that either go directly through the repository block, or adjacent to it. The left-hand (direct-intrusion) branch then divides to reflect intrusions that either destroy waste packages and subsequently entrain their contents to the surface (dispersing them either as lava flows or as ash plumes), or intrusions that encapsulate the waste packages after causing them to fail. In the latter case, the waste can contribute to a greater radionuclide source term for transport of contaminants by groundwater flow.

The right-hand (indirect-effects) branch of the FEP diagram depicts changes that can occur in the groundwater flow patterns in both the unsaturated and saturated zones as a result of a dike intrusion near the repository. An intrusion may be located adjacent to the repository block, or beneath it. Depending on whether the dike acts as a flow conduit or flow barrier, and whether it is in the unsaturated or saturated flow fields determines the potential effects. A few are illustrated in Figure 6.10-1; water-table rise, concentration of contaminants in the SZ, and lateral diversion and ponding in the UZ.

Figure 6.10-2 shows more detail of the direct-intrusion FEPs. The branch expanded in the Figure considers the consequences of an intrusion where the gasses in the magma exsolve below the repository, creating ash, pyroclasts and aggressive vapors. If the magma conduit intersects a waste package (indicated as path 1 in the Figure), such an environment is expected to rapidly cause structural failure of the container. When the waste form is exposed to the magma/ash flow, it can be entrained; the amount so carried in the ascending column is a function of the size of the contaminant particles and the density of the flowing material. Similarly, the dispersion of contaminants in the ash plume is dependent on factors such as wind speed, particle size, etc. The details of the component models (e.g., timing of waste-package failure, and entrainment and dispersion mechanisms) must be supplied by the respective subsystem analyses.

Path 2 in Figure 6.10-2 illustrates the scenario for potentially increasing the radionuclides available for transport by groundwater. Magma filling a drift may not be as erosive as that flowing to the surface, so the waste form is more likely to remain inside the degraded waste packages. Volatile components of the waste can be boiled off and condensed elsewhere in the drift. As the magma cools, it encapsulates the waste; thermal and mechanical stresses can crack the encapsulating rock. Eventually, groundwater can return to the drift and reach the exposed waste through the fractured basalt. The dissolved waste and/or condensed volatiles can increase the amount of contaminants available to be transported by groundwater flow.

There are several fundamental unknowns associated with the effects of a dike intrusion outside the repository. For example, an intrusion might act as a barrier to flow, or as a conduit (see Figure 6.10-1); furthermore, over long time periods the dike may change from one flow effect to another. If an intrusion occurs along existing structures that currently are thought to influence flow, the disturbance might be modeled as enhancing the currently observed effects. Given the uncertainties in our phenomenological understanding of how alterations to the flow field might occur, analyses might be done by assuming that an intrusion has caused flow perturbations, and calculating the impact on performance.

The details of the models for intrusion plumbing, enhanced waste-package degradation, waste entrainment, airborne dispersion, and other effects must be developed by the appropriate subject-matter experts. The information provided in the PHA report will also be applied to model development. In the process of doing so, additional or replacement scenarios may be studied if they appear to have greater consequence or higher probability.

6.10.4.2 Nuclear Criticality

Figure 6.10-3 shows the overview of criticality scenarios. Regardless of the location of a potential critical configuration — in-package, near-field, or far-field — the initiating processes must include degradation of the waste package to failure, and introduction of water into a breached waste package. Additionally, several other conditions must obtain before a criticality is theoretically possible. These include a geometry of the fissile fuel that minimizes neutron leakage, the absence of neutron absorbers that can reduce the number of neutrons available to cause fissions, and the presence of a neutron moderator to maximize the probability of fission reactions.

There is sufficient fissile material in most waste packages to meet the fuel requirement for a critical configuration, but outside the container some form of re-concentration mechanisms is needed before there would be sufficient fissile material. The waste package incorporates neutron absorbers that must be removed to permit the formation of a critical configuration; in the near and far fields, the transport and re-concentration processes may separate absorbers from fissile material.

The FEP tree shows the branches that can lead to criticalities in various locations. The various FEPs necessary to remove absorbers, re-concentrate fissile material, or provide moderator or favorable geometry (as applicable to the type of criticality under consideration) are indicated.

To achieve these conditions inside a waste package depends on the type of waste present. Commercial spent nuclear fuel (CSNF), composed of Zircaloy-clad reactor fuel rods in fuel assemblies, is designed to support criticality in the presence of water — provided the neutron absorbers are absent. This type of waste is quite resistant to mechanical collapse or chemical degradation, so FEPs that describe the removal of the absorbers from a waste package containing water are applicable to this type of criticality. Alternatively, DOE spent fuel (aluminum-clad) is more likely to degrade before the waste-package neutron-absorbing internal structures, so FEPs that describe accumulation of fissile material in the bottom of a water-filled waste package are applicable to this type of system. These branches are illustrated in Figure 6.10-4 (along with a few other FEPs potentially leading to critical configurations). The path "F" shown in the Figure leads to near-field criticalities.

Because of the potential availability of fissile material from several nearby waste packages, and possibly relatively high concentrations of fissile-material solutions, FEPs for near-field critical configurations reflect a number of alternative geometries. These are illustrated in Figure 6.10-5. The FEP diagram begins with failure of the waste-package bottom, which permits water containing fissile material (and possibly the neutron absorbers) to flow out of the package and onto the drift floor. The concrete and/or crushed tuff comprising the drift floor can potentially create a favorable geometry by channeling flow, provide neutron reflectors that enhance neutron multiplication, separate fissile material from absorbers by differential sorption, or re-concentrate fissile material by precipitation of solutes or filtration of colloids. Some of these FEPs are shown in Figure 6.10-5, each leading to a potential critical configuration. Additionally, the path "I" is shown for potential far-field critical configurations.

Re-concentration of transported solutes or colloids is the most important factor in the formation of potential critical configurations in the far field. In nature, ore deposits form when a dissolved species (such as uranium) is reduced in its oxidation state, which causing precipitation. Reducing agents include organic materials, such as carboniferous deposits, and groundwaters from deep sources. Localized reducing conditions often cause "roll fronts" where relatively high concentrations of minerals can accumulate (Bailey and Childers, 1977). Reducing locations are postulated in the FEPs shown in Figure 6.10-6 as causing concentrations of uranium to accumulate. Plutonium is considerably less soluble in groundwater than uranium, so the most likely method for its transport is as colloids or pseudo-colloids. Re-concentration mechanisms for colloids include filtration by clays, or trapping in fractures.

The final selection of FEPs to be analyzed will depend on further analyses to ensure that all the required conditions for criticality are present. In the waste package, this will consist primarily of determining mechanisms to remove neutron absorbers from the waste package; for the near and far fields, it is necessary to establish the feasibility and conditions for re-concentration.

6.10.4.3 Seismicity

The scenarios to be analyzed for seismicity are illustrated in Figure 6.10-7. The two top-level FEP-tree branches for either a new or old fault activated in the repository block cover all the potential seismic effects — rockfall, fault displacement damage, flow-path alteration, and water table rise. The top-level branch "Regional Coupling" is a source for rockfall and water-table rise. Rockfall is modeled as a consequence of seismic disruptive events, but it is expected to occur more frequently as a result of normal thermo-mechanical repository stresses. Thermo-mechanically induced rockfall will be included in the base case.

The PA implications of a new fault developing in the repository (*vs.* reactivation of an old fault) is that waste packages will not be located in an existing fault zone, so damage from fault displacement is not expected to occur in the latter case. Rockfall has the effect of enlarging the drift diameter and potentially removing sufficient amounts of thermally altered rock from the flow path to the drift to change the nature of water flow into the drift. Other examples of flow-path alteration include seismically induced changes in stress states that can open or close fractures. Permanent water-table elevation change can potentially shorten the transit time for contaminant transport by causing more of the flow path to be saturated.

6.10.4.4 Human Intrusion

The scenario analyzed for human intrusion will follow the recommendations of the NAS panel on Yucca Mountain standards (NRC-NAS, 1995). This scenario assumes that a drilling incident has punctured a waste package, and that drilling operations continue to the water table. The scenario which allows waste from the punctured container to fall directly into the saturated zone. We assume that the entire contents of one waste package reach the saturated zone as solids or as solutes carried by drilling mud, and the waste can then be dissolved and transported by the available groundwater.

6.10.5 Abstraction Approach and Assumptions

The models for use in TSPA-VA for volcanism, seismicity, and human intrusion have not been fully developed. The models will be completed in the early part of FY 1998. Therefore, a listing and discussion of modeling assumptions cannot be provided at this time.

Therefore, a listing and discussion of modeling assumptions cannot be provided at this time. A full discussion of modeling assumptions will be provided as the model development is completed and reported in TSPA-VA. Additional modeling assumptions will be documented as modeling is completed in 1998, and will be shown and discussed in the TSPA-VA.

6.10.5.1 Nuclear Criticality

For criticality, the initial steps for model development and abstraction were begun in FY 1997:

- Important issues for characterizing criticality were identified by a group of experts at the criticality workshop in March, 1997 (CRWMS, 1997b).
- The important issues were incorporated into FEP diagrams and described in a report (Barnard et al., in preparation). The results of preliminary calculations have been used to select a few of the FEP-diagram paths (i.e., scenarios) as being potentially of relatively high consequence and/or high probability.
- Further model development for the selected scenarios will be completed in early FY 1998. Scoping analyses (such as geochemical reaction-rate calculations with the code EQ3/6) are being performed for the appropriate FEPs. The Waste-Package Development organization of the M&O has completed several calculations of the neutron multiplication

factor (k_{eff} – a measure of criticality) (CRWMS, 1996b). The other boundary conditions, such as water flow rate and amount, waste-package corrosion modes, absorber dissolution rate are being selected, based on inputs from other abstraction and testing activities.

- For the abstraction effort and the TSPA-VA analyses, an "efficient" method of evaluating the impact of a criticality event on total-system performance is to follow a three-step analysis:
- *Assume that a critical configuration exists, and calculate the impacts.* For example, assume that the contents of one waste package containing CSNF of a given burnup and age have formed a critical configuration with k_{eff} of 1.0. Based on the FEPs of the scenario, assume that the optimum conditions for criticality exist. For these conditions (e.g., the geometry, the amounts of fuel, moderator and neutron absorbers present), estimate the duration of the criticality and the number of fissions that would occur. Calculate the fission-product and actinide inventories created by the criticality to see if they represent a significant modification to the existing radionuclide inventory. One of the factors that determines whether the additional inventory is a significant perturbation depends on the time at which the criticality event occurs. If the perturbation to the inventory warrants further investigation, then do the next step.
- *Determine the geologic processes and conditions necessary to create the critical configuration.* By modeling the processes, rates, and timings of the FEPs that must occur to create the critical configuration, additional information can be developed that may change the parameters of the criticality. By recalculating k_{eff}, the power and duration of the criticality, and the resulting radionuclide inventory, the significance of the criticality to repository performance (in the form of an alteration to the radionuclide inventory) can be reevaluated. Again, if the criticality appears to cause a significant perturbation to the inventory, the final step can be undertaken.
- *Perform a TSPA analysis using the modified inventory.* The radionuclide inventory becomes the source term for groundwater flow and transport analyses and dose calculations. Impact of the criticality on repository performance can be directly reported as an increase in dose or releases as a function of time, or other measure.

By using this three-step method, unnecessary analyses will not be done on scenarios that have no PA impact.

6.10.5.2 Igneous Activity

Preliminary investigations of some of the aspects of igneous activity in the Yucca Mountain area were completed in prior years (Valentine, 1995; CNWRA, 1996). To model the direct-intrusion problems for TSPA-VA, the following model components are planned to be developed in FY 1998:

- plumbing of intrusions, including whether eruptions are monogenetic or polycyclic,

- nature of igneous activity, especially the depth of exsolution of magmatic gasses and hydrovolcanic effects,
- volume of intrusions and interactions between intrusive magma and repository workings (including extent of magma flow down drifts, extent of thermal effects on waste packages and adjacent rock),
- mechanisms, rates, and extent of waste-package degradation by magma and magmatic constituents,
- mechanisms for entrainment of waste, considering magma-flow properties, waste structure, and waste-particle size and density,
- seismic effects associated igneous activity, and the acceleration of waste-package degradation that seismicity could cause,
- mechanisms and extent of dispersal of contaminants in ash plumes,

The Probabilistic Vollcanic Hazard Analysis (PHA) study provides distributions of probabilities of occurrence for an igneous intrusion intersecting the repository footprint and continuing to the surface. Additional work must be done to develop probability distributions for specific interactions between intrusions and the repository (such as are listed above), and for intrusions outside the repository (for use with the indirect-igneous studies).

The same general scheme that is described above for criticality will be used for the volcanic analyses — effects of igneous intrusion will be calculated, and their effect on overall system performance will be evaluated. A full listing and discussion of modeling assumptions will be provided as the model development is completed and reported in the TSPA-VA.

6.10.5.3 Seismic Activity

Rockfall will be modeled as having two effects on waste packages. The first is direct mechanical damage from impact (most likely to be important for waste packages that are already corroded). The second is the change in unsaturated flow conditions that can occur from rockfall. As a result of thermo-chemical effects, the rock of the drift wall can change its permeability due to mineralogical changes. It is postulated that a relatively impermeable "rind" will form on the drift walls that may reduce or divert water flow away from the drift. Extensive rockfall can remove this altered rock. Additionally, rockfall debris around the waste packages can provide a capillary path for water to reach the waste packages. The details of these models will be developed in early FY 1998. These effects can be seen to be perturbations on the base-case water-contact modes, corrosion processes, and waste-form-mobilization models. They will be therefore included in TSPA-VA as sensitivity studies on the appropriate models, and the PA effects expressed as changes to the base case.

Water-table rise will be incorporated in TSPA-VA using a seismically driven model (Arnold, in press) as a sensitivity study on combined UZ–SZ flow and transport. The model predicts different amounts of water-table elevation change for different types of faulting, so a range of elevations will be used in the transport sensitivity studies. Additional modeling assumptions will be documented as modeling is completed in 1998, and will be shown and discussed in the TSPA-VA.

6.10.5.4 Human Intrusion

Abstraction of this scenario for TSPA-VA involves applying a model for dissolution of the waste form under saturated conditions and then calculating the transport of the mobilized contaminants. These calculations will be done separately from the base case. To provide an estimate of the impact of this scenario on overall repository performance, the doses from the human-intrusion case can be compared with the base-case doses.

6.10.6 Incorporation of Disturbed Analyses into Base Case

As mentioned previously, the disturbed effects will be calculated separately and the impacts on repository performance will be determined by treating the effects as perturbations to base-case TSPA components, such as the radionuclide source term for groundwater flow and transport. Where this approach is not directly applicable (as for direct volcanic surface releases), the risk (consequence times probability of occurrence) distributions will be incorporated into the overall base-case results to show the impact. To summarize, the following types of performance assessments are planned:

- **Igneous activity:** (1) direct mechanical transport to the surface, with performance impacts from surface-contact doses and airborne doses; (2) increase in the radionuclide source term at the repository for groundwater flow and transport through the UZ and SZ arising from magmatic disturbance, with performance impacts from possible increases in dose at the accessible environment compared with the base case; and (3) modification of the SZ flow and transport processes between the repository (contaminant source) and the accessible environment due to an igneous intrusion, with performance impacts from possible increases in dose at the accessible environment compared with the base case.
- **Nuclear criticality:** (1) in-package critical configurations causing increases in the groundwater-flow radionuclide source term at the repository, with performance impacts from possible increases in dose at the accessible environment compared with the base case; (2) near-field critical configurations causing increases in the groundwater-flow radionuclide source term at the repository, with performance impacts from possible increases in dose at the accessible environment compared with the base case; and (3) far-field critical configurations causing the creation of groundwater-flow radionuclide source terms away from the repository closer to the accessible environment, with performance impacts from possible increases in dose and different radionuclide contributors to the dose at the accessible environment (compared with the base case).

- **Seismic activity:** (1) increase in the radionuclide source term at the repository for groundwater flow and transport through the UZ and SZ arising from rockfall and ground-motion disturbances, with performance impacts from possible increases in dose at the accessible environment (compared with the base case); (2) alteration of groundwater-transport of radionuclides from the repository due to transient and permanent water-table elevation rise, with performance impacts from possible increases in dose at the accessible environment (compared with the base case); and (3) modification of the SZ flow and transport processes between the repository (contaminant source) and the accessible environment due to faulting, with performance impacts from possible increases in dose at the accessible environment compared with the base case.
- **Human intrusion:** potential increases in dose at the accessible environment from transport of radionuclides mechanically transported to the SZ by drilling, with performance impacts from possible increases in dose at the accessible environment (compared with the base case).

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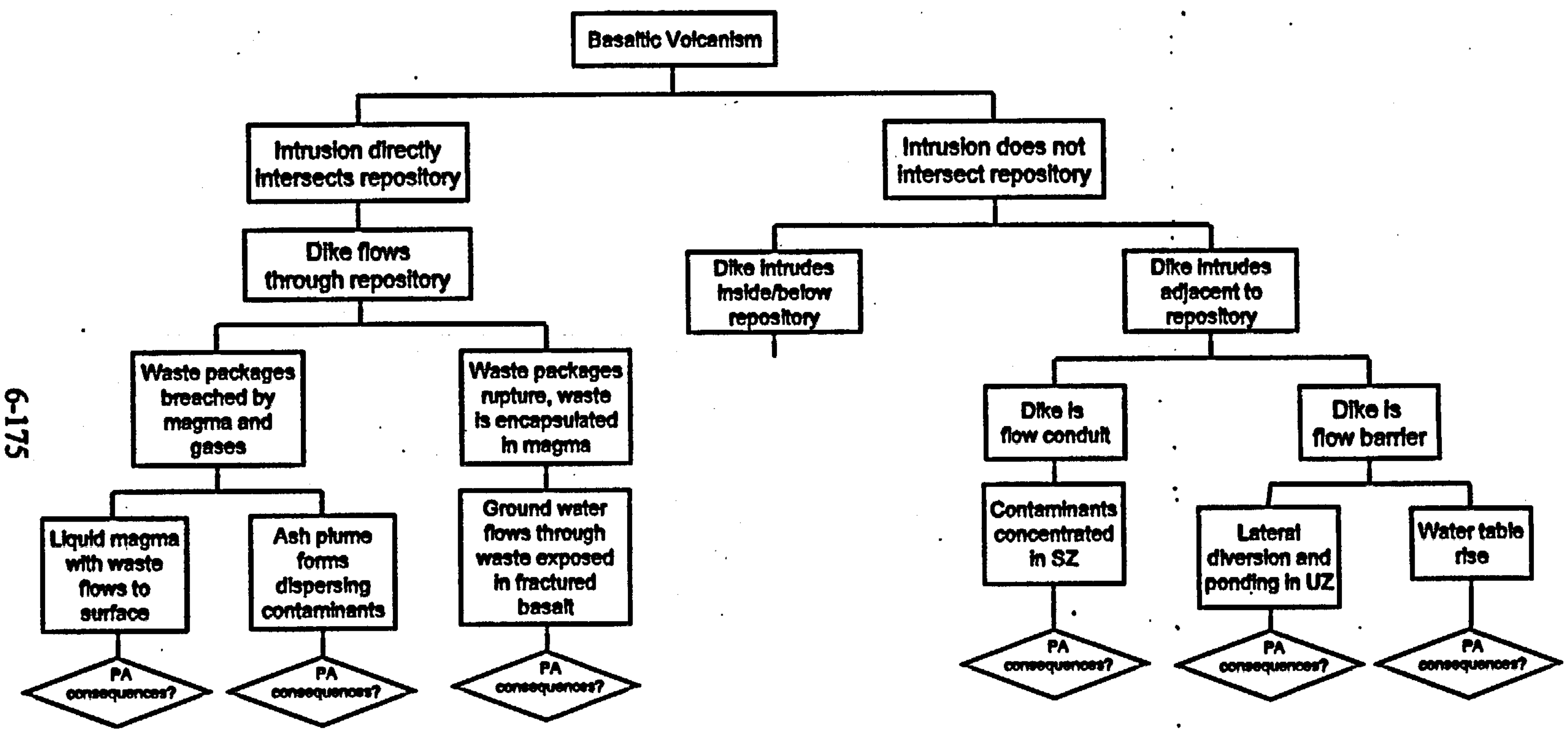


Figure 6.10-1. Top-level FEP diagram for igneous activity

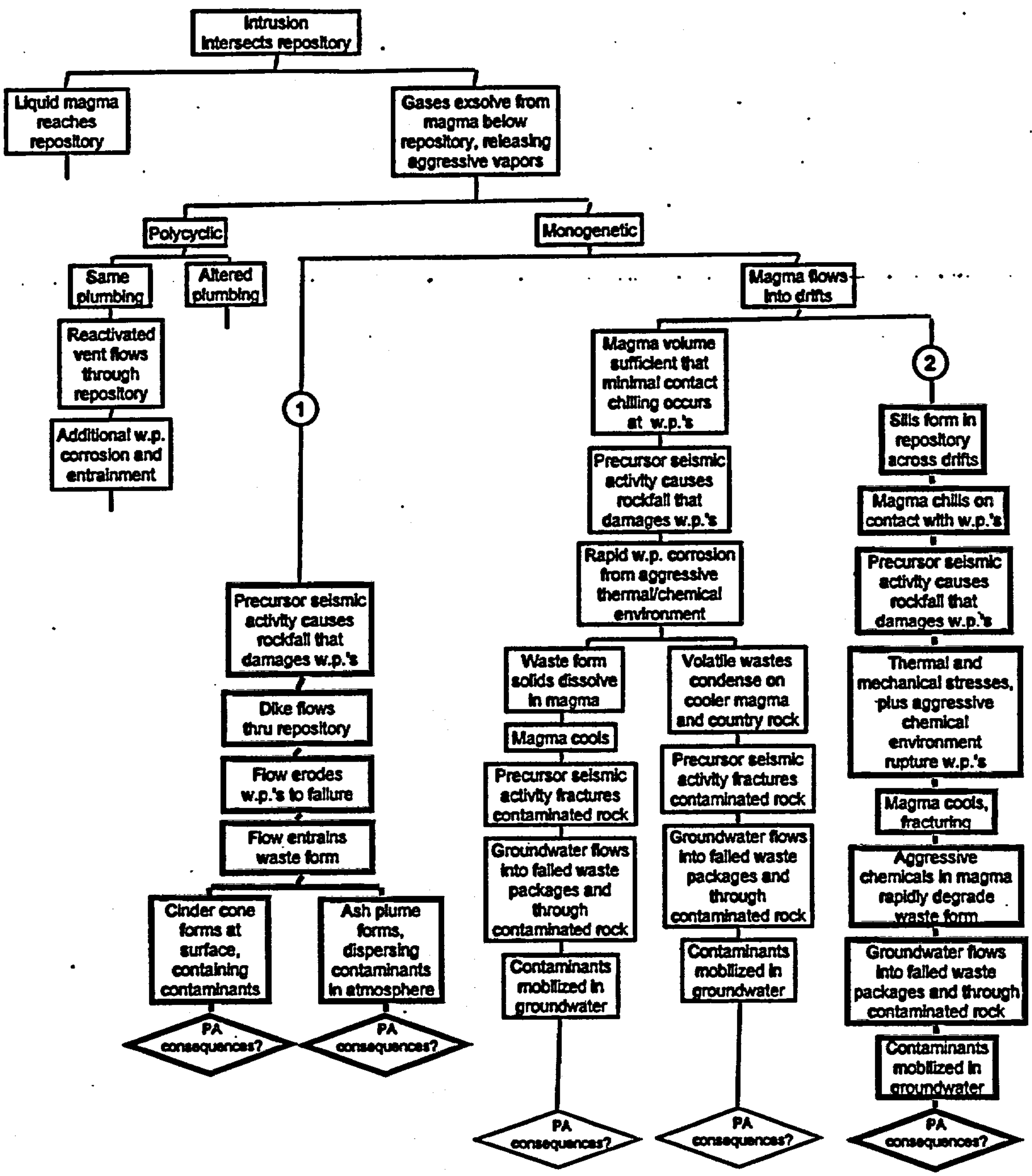


Figure 6.10-2 FEP diagram for direct igneous intrusions into repository

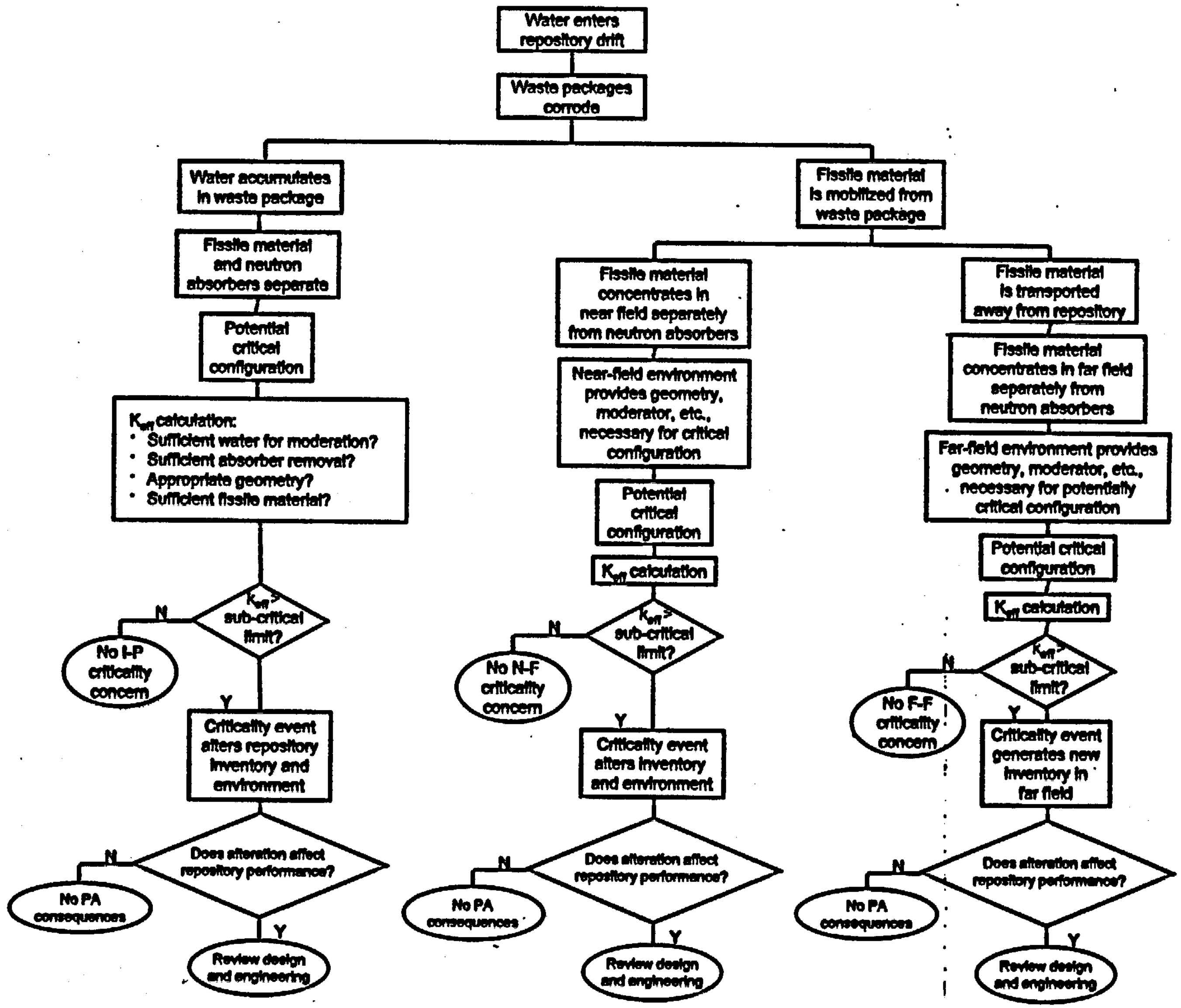


Figure 6.10-3 Top-level FEP diagram for nuclear criticality

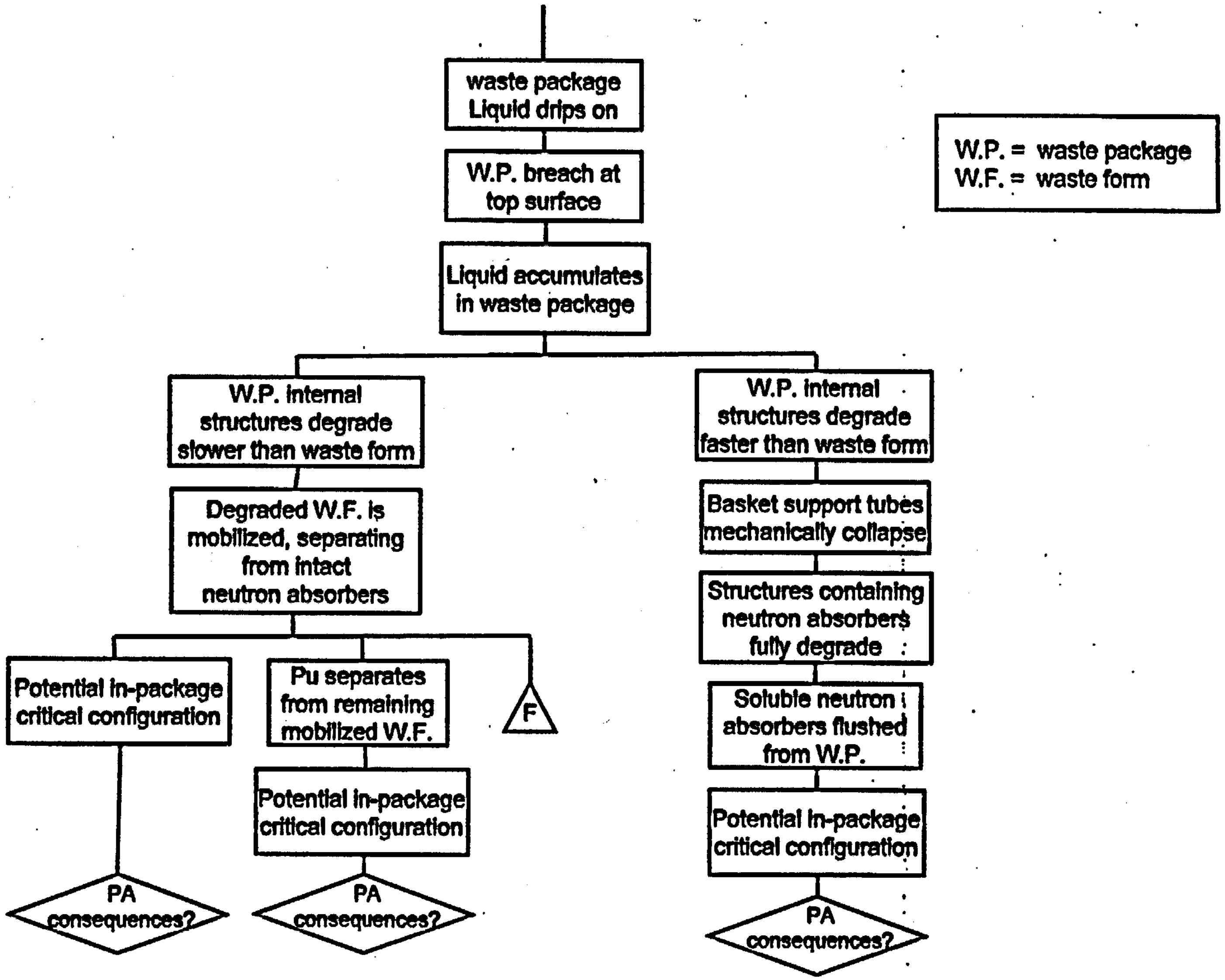


Figure 6.10-4. FEP diagram for in-package critical configurations

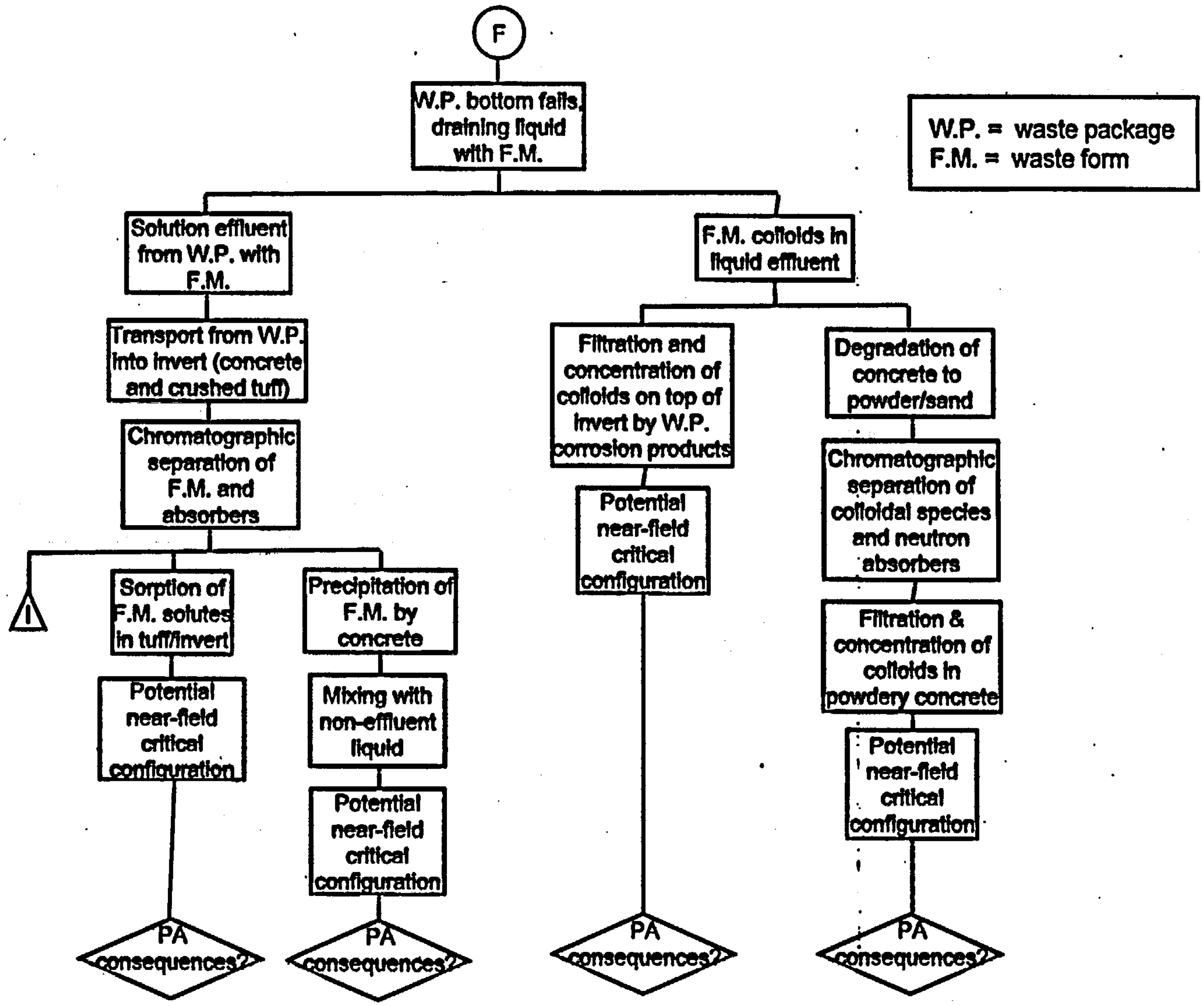


Figure 6.10-5. FEP diagram for near-field critical configurations

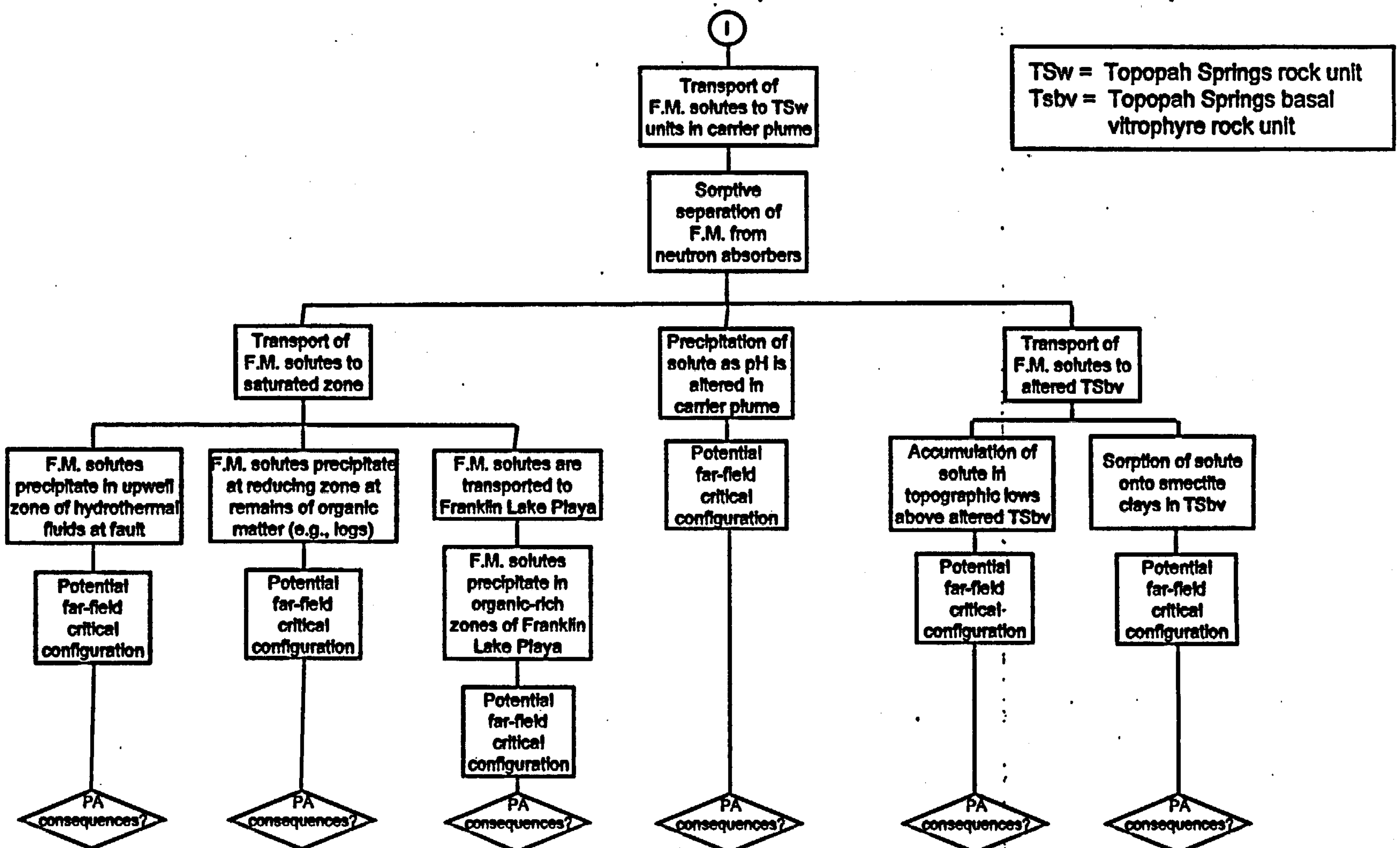
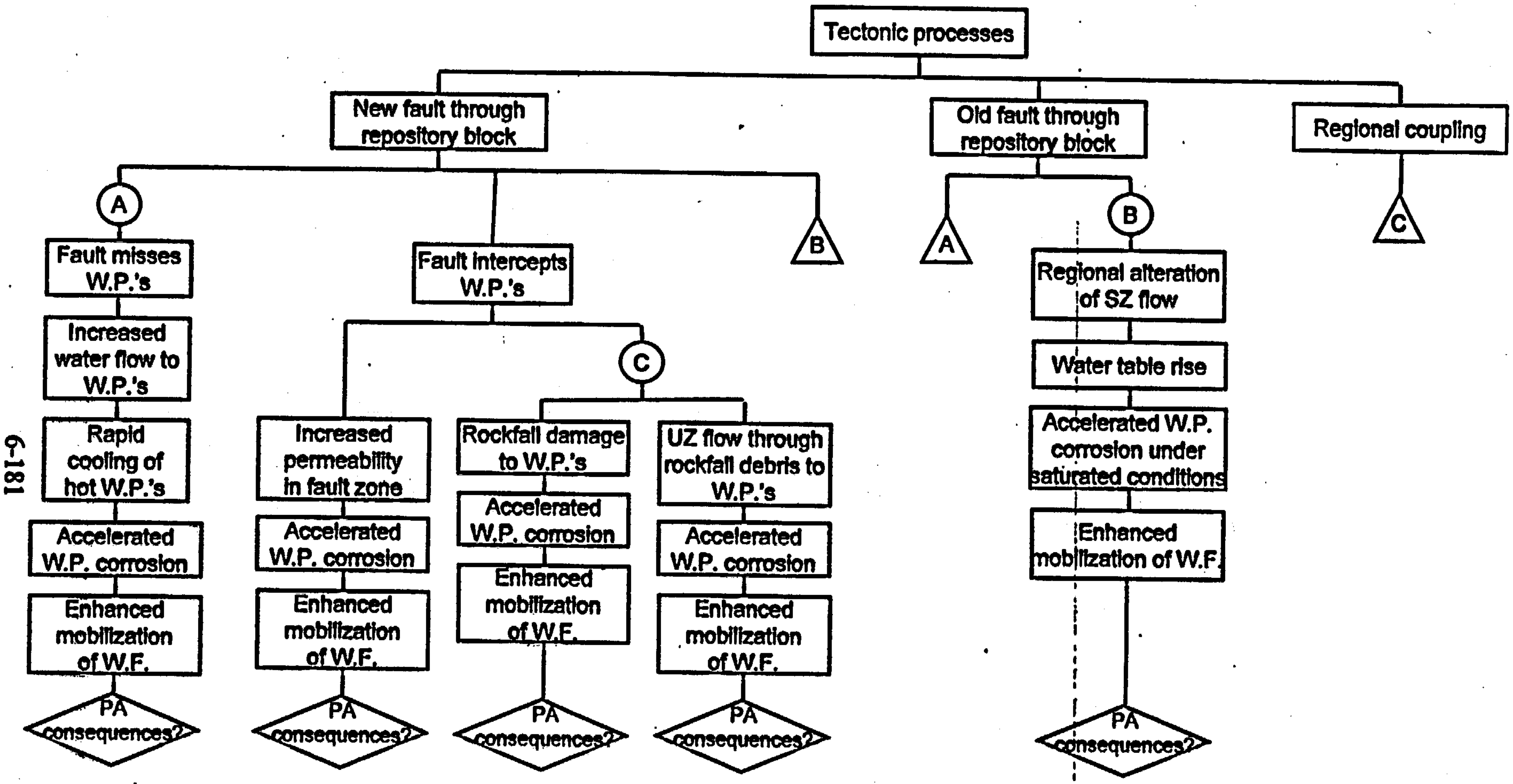


Figure 6.10-6. FEP diagram for far-field critical configurations



W.P. = waste package
W.F. = waste form
UZ = unsaturated zone
SZ = saturated zone

Figure 6.10-7. Top-level FEP diagram for seismic disturbances

7.0 IMPLEMENTATION OF THE BASE-CASE MODEL IN THE TSPA-VA CODE

S. David Sevougian, Michael L. Wilson, Jerry A. McNeish, Jack H. Gauthier, Rob Howard

7.1 INFORMATION FLOW IN TSPA-VA

Having discussed in detail in Chapter 6 each of the major components and models of the TSPA-VA, including the process models, primary abstraction assumptions and approaches, and base-case and sensitivity cases for each component, this chapter will look at the integrated picture again, i.e., how to fit all the pieces back together into one coherent model and code. In order to lay the groundwork for the code architecture, we first review the information flow between the various models (already briefly touched upon in Section 4.3) and also the major types of abstractions that form the underpinning for the overall model and code architecture (already briefly touched upon in Section 5.3). After the discussion of the model and code architecture, there is a general discussion of uncertainty and variability in TSPAs, and a specific discussion of uncertainty/variability as it will be incorporated in TSPA-VA and as it affects the definition of the base case and sensitivity cases and the definition of the "most probable" repository behavior (see also Section 5.4 for an overview of uncertainty/variability as if affects the TSPA-VA general approach and method). Finally, this chapter concludes with a discussion of alternative repository designs that will be considered in TSPA-VA and the methods of sensitivity analysis (uncertainty and importance analysis) that will be used to determine the most influential parameters and models on overall system performance.

7.1.1 Effect of Abstractions on Information Flow

PA Pyramid. Because of the complexity, uncertainty, and variability of the repository and its components, involving a variety of coupled processes (thermo-hydrologic-chemical-mechanical) operating in three spatial dimensions on a variety of different materials (e.g., fuel rods, waste canisters, invert, host rock, etc.)and changing over time, it is generally necessary to make some simplifications to the detailed process-level models. This is particularly true in total system performance assessment, which has a significant component of probabilistic risk analysis (PRA). The general PRA approach is appropriate because of the inherent uncertainties in predicting physical behavior many thousands of years into the future in a geologic system whose properties can never be fully characterized deterministically. In particular, there is always a degree of uncertainty and variability in natural geologic systems, which when carried forward into predictions of future behavior, requires a probabilistic method. Thus the detailed models of physical-chemical processes would need to be run hundreds of times to generate many possible realizations of the future behavior. Because the process-level models are restricted to a finite amount of computational resources and time, simplifications ("abstractions") are generally necessary.[1]

[1] For the purposes of TSPA, the word *abstraction* is used to connote the development of a simplified/idealized process model that reproduces or bounds the results of an underlying detailed process model.

Based on this abstraction or simplification paradigm, the overall conceptual framework for information flow within the Total System Performance Assessment (TSPA), as embodied in the TSPA Model Hierarchy, is shown in Figure 7.1-1. This figure indicates a continuum of information and models from the most basic, detailed level up to the level of the total system model. The data and conceptual models rest at the base of the pyramid and feed into detailed process-level models. These process-level models may be simplified or abstracted, if necessary, because of computational constraints or because of lack of information. The resulting subsystem models may have a one-to-one correspondence to the detailed process-level models or may represent a combined model covering several aspects of the overall system. These models may also be simplified if necessary to feed into the total system performance assessment model at the top of the pyramid. The total system model simulations can then be performed in a computationally intensive probabilistic framework because of the simplifications which have been made in representing the process models. (Examples of various "subsystems" include the engineered barrier system, the unsaturated zone, and the saturated zone. In this sense, the defining boundaries of these subsystems are clearly spatial boundaries, and the primary form of information transfer between the subsystems is radionuclide mass flux.)

Several key factors must be observed for this model simplification process to accurately represent the performance of the overall system. First, information passed up the model pyramid must be self-consistent. For instance, an infiltration flux used to generate flow fields from the detailed unsaturated-zone process model, must be used in all subsequent analyses based on those particular flow fields. In particular, it must be used when calculating seepage flux into the drift and when calculating thermohydrologic response (temperature and relative humidity) in the near-field environment. Second, and this is a key requirement on the abstraction process in general, the parameters in the detailed models which most affect performance must be appropriately represented in the subsequent subsystem and total system model. In particular, it is expected that all details of the process models will not need to be carried forth to the total system models because they may not directly affect performance; however, those key parameters or processes which significantly affect performance must be properly represented in any simplification included in the total system performance assessment. Specifically, since we believe the more complex models to be more accurate (or at least that they have a higher degree of spatial-temporal resolution), we want the simple model responses to "bound" the more complex model responses, i.e., to always give equal or higher values for the doses or risks to the public.

<u>Overall information flow diagram</u>. As described previously in Section 4.3, and shown in Figure 4.3-1, the overall information flow in TSPA-VA is quite complex. Each piece of information or model developed must be appropriately represented in the performance assessment analyses. The flow of information starts from test data and the corresponding interpretation and documentation of these data; then to the use of process-level models to synthesize the available test data and other information into a consistent representation of the relevant processes affecting waste isolation and containment; to the abstraction of results from these process-level models in the form of response surfaces, table look-ups, or other functional relationships; and finally, to the total system performance assessments themselves.

Figure 7.1-2 shows an upper-level view of the main sources of information for the total system performance assessment. The figure is subdivided into four major categories: (1) Information, (2) Process Level Model, (3) Process Level Model Abstractions, and (4) Total System Performance Assessment. These categories represent major steps in the analyses required for TSPA-VA. The Information category includes all of the data being collected and already collected for the project: information on the repository and waste package design, the materials used in that design, the site hydrologic and geochemical characteristics, and the current biosphere. The figure indicates how the information sources feed the detailed process level models. There are eight key process level models which are being developed and incorporated into the performance assessment analyses: a waste-form degradation/mobilization model, waste-package degradation models, mountain- and drift-scale thermohydrologic models, an unsaturated-zone flow model, an unsaturated-zone transport model, a saturated-zone flow model, and a biosphere model based on the current population in the general vicinity of the repository. Each of these process models will provide information to be abstracted or simplified into the total system performance assessment model. In general, the abstractions are response surfaces (multi-dimensional tables) that will be input to the TSPA model. The key abstractions are presented in the figure and listed in Table 7.1-1. Table 7.1-1 is similar to Table 4.3-1, but also lists the computer codes to be used for each abstraction.

The numerous computer codes which will be implemented in TSPA-VA are shown schematically in Figure 7.1-3. The code linkages are indicated with an arrow, generally feeding information or abstractions to the main integrating code, RIP in the center of the figure. TOUGH2 will be used to generate flow fields for the transport calculations (FEHM-RIP) and parameter sets for the thermohydrology simulations (NUFT and TOUGH2). The waste package degradation model WAPDEG, will receive information from the thermohydrology and the near field environment geochemistry evaluations. Near field environment geochemistry evaluations will be conducted with both EQ3/6 and AREST-CT. These various code linkages and the types of abstractions expected are discussed in detail in subsequent sections.

7.1.2 Data Integrity

The TSPA-VA analyses will be conducted and documented following a formalized application of good scientific and engineering practices. This approach will include reporting and tracking techniques which provide for traceability and transparency of all data, models, input, and output. For design and site information, QAP-3-12 *Transmittal of Design Input* will be used to obtain and track the information.[2]

Within PA, the analyses conducted will be documented for traceability. All data sources will be recorded. Input files will indicate which version of configured software was used for the particular

[2] QAP- 3-12 is a formalized information tracking and control procedure currently being used on the Yucca Mountain Project to trace and document the transfer of information amongst various organizations. It implements a part of the OCRWM Quality Assurance Requirements and Description (DOE/RW-0333P Revision 7) for interface control.

analysis. Software will be managed in a controlled configuration management environment, such as RCS for Unix operating systems (Tichy, 1985). Output files and plots will also indicate the input file used, the version of the software used, and the date and time of the analysis. Modules used as add-ons to the RIP code will also be controlled and noted on the output files.

7.1.3 Quality Assurance

Since the TSPA is intended to be used as part of the 2002 planned License Application's evidence of the proposed repository's ability to meet regulatory safety criteria, and since even now it provides input to the repository design process and site-characterization activities, the level of documentation and traceability of inputs, assumptions, and decisions needs to be consistent with the level of documentation supporting engineering design and site characterization. The rigor and associated level of documentation required for design work and site characterization is prescribed primarily by the OCRWM Quality Assurance Program. Performance Assessment activities and work processes are different than those in design or site characterization. Therefore, although consistency must be ensured with the design and site-characterization procedures, many of those design/site procedures will be inapplicable and other procedures will need to be developed specifically for performance assessment activities. Development of the Quality Assurance Procedures for Performance Assessment is currently underway. It is expected that the Total System Performance Assessment for Viability Assessment will be prepared, reviewed, and approved in accordance with an approved quality assurance procedure.

One of the key aspects of establishing a controlled reference TSPA model is providing confidence that the TSPA analyzes the natural system described by Scientific Programs Operations and the configuration of the engineered system documented by Engineering and Integration Operations. In order to accomplish this, the technical information that is exchanged among Performance Assessment, Engineering and Integration, and Science must be managed and well documented. The current system used by Engineering and Integration to manage technical information exchanged between organizations is described by QAP-3-12, *Transmittal of Design Input*. Currently the design input needed for TSPA-VA is being controlled via QAP-3-12, which will help ensure that the Performance Assessment organization receives current information and that inputs are auditable and traceable to their source. This system may not be completely adequate to support the Performance Assessment activities and will be re-evaluated to better suit Project needs as the design and its associated performance assessment mature. It is possible that NLP-3-34 *"Interface Control"* (currently in draft) will be implemented to document bi-lateral agreement between Performance Assessment and interfacing organizations on base cases used for TSPA-VA.

In addition to the input control features described above, Performance Assessment plans to make use of YAP-SIII.3Q, *"Processing of Technical Data on the Yucca Mountain Site Characterization Project"* and the *Geographic Nodal Information Study and Evaluation System* (GENISES), to the extent practical for obtaining and tracking data used as input to the TSPA. This will help ensure that data used as input for TSPA is identified in a manner that facilitates traceability to associated documentation as well as being traceable to its qualification status as required by the OCRWM

Quality Assurance Requirements and Description (DOE/RW-0333P Revision 7). It should be noted however, that the information contained in these technical databases is not a complete set of the data required for TSPA-VA. Therefore additional data may be taken from the open literature, or assumed values for some parameters may be used in TSPA; in these cases, the bases for the assumed values or reference to literature will be explicitly stated.

7.2 TSPA-VA MODEL AND CODE ARCHITECTURE

7.2.1 TSPA-VA Model Architecture

Underlying the architecture of the overall TSPA computer code, is the overall model architecture, i.e., how the various spatial-temporal representations of the relevant physical-chemical processes are linked together. This subsection on model architecture describes the basis for these linkages as implemented in TSPA-VA, and is predicated on the need for model abstractions as described in the previous section and in Section 5.3.

7.2.1.1 Model Architecture as a Function of Domain- and Process-Based Abstractions

Based on the main repository components and processes depicted in Figures 4.1-1 to 4.1-3, the primary basis underlying the performance-assessment model architecture is a "domain-based" or spatial abstraction. That is, there is a natural division of the repository system into a series of sequentially linked spatial domains, e.g., the waste package, the emplacement drift, the host rock "near" the drift, the unsaturated zone between the drift and the water table, the saturated zone, etc. This division works best from the standpoint of radionuclide *transport*. In particular, the ultimate goal of TSPA is to track and predict radionuclide transport from the waste-form domain to the biosphere domain (and all intervening spatial domains) over future time, while including some estimate of the uncertainty in the predictions. The TSPA-VA model architecture uncouples the domains (i.e., ignores feedback, which is generally a valid assumption for transport) except in the one case of near-field diffusion where gradients are moderated over time as geosphere concentrations become non-zero, which is address though a temporally varying input parameter, and becomes a sequential calculation in which each domain-based transport model may be run in succession, with output-mass versus time from an upstream spatial domain serving as the input-mass versus time for the spatial domain immediately downstream. ("Upstream" and "downstream" refer to the direction of mass flow or energy flow.)

Overlying this spatial-domain-based *transport* architecture is another level of discretization of the entire system: one based on decoupling of physical processes. In particular, the feedback/coupling between certain processes is assumed to be weak: entropy/energy of the processes is assumed to flow primarily in one direction. For example, it is assumed that the thermohydrology (or just hydrology, after the thermal pulse decays) establishes and controls the liquid flux (Darcy velocity) field for the transport-based models, but that transport-induced processes, such as mineral precipitation, only weakly feedback to thermohydrology or hydrology. In this case the mineral precipitation (which reduces rock porosity) is assumed to only weakly affect the rock permeability and hence the liquid-phase velocity field. These other physical processes (i.e., other than transport) may also involve "domain-based" abstractions. For example, usually there are separate process-level models for "drift-scale" thermohydrology (at the scale of meters or tens-of-meters) compared to "site-scale" or "mountain-scale" thermohydrology (on the order of hundreds-of-meters). The correct coupling of these domains is a key piece of the model and code architecture to be discussed below.

The assumption of energy/entropy flowing one way between physical processes implies that the "upstream" process may be solved independently of the "downstream" process; however, if the fluxes and/or phenomenological coefficients of the upstream process are time-varying and appear in the equations of the downstream process, then the downstream process equations must be solved simultaneously with the upstream process equations. An example is that for a transient (time-varying) flow field (Darcy velocity), the transport equations must be solved simultaneously with the flow equation; however, the flow equation could be solved independently of the transport equations. A useful abstraction in this regard is the assumption of steady-state flow. This could be termed a temporal decoupling of flow and transport that depends on a relatively rapid time constant for changes in fluid velocity compared to transport of radionuclides through the system. The main advantage of this from a TSPA perspective is that the numerical solution of the transport equations (based on a linear K_d model for chemical processes, and to a lesser extent on the use of a particle tracker rather than a finite-difference method) is generally much faster than the solution to the two-phase flow equations. Thus, the flow fields can be solved (and a "library" of them developed as a function of various parameter uncertainties) well ahead of the running of the overall TSPA-VA model. These flow fields may then be imported into the particle tracker for transport which can be run very fast over a range of uncertainty in certain transport parameters, such as K_ds, matrix diffusion, and dispersion.

The overall TSPA-VA model architecture for coupling and information transfer between the various domain/process-based models (both the detailed and abstracted models) is shown schematically in Figure 7.2-1. The sequential order for information flow is: Site-Scale Thermohydrology → Drift-Scale Thermohydrology → Waste-Package Degradation → Waste-Form Degradation → EBS Transport → Unsaturated-Zone Flow/Transport → Saturated-Zone Flow/Transport → Biosphere Transport. This sequential order of processes and domains follows the logic described above, wherein the input boundary conditions of one process/domain are provided by the output from the preceding process/domain. For example, the time-dependent repository-scale percolation flux q(t) is derived from the site-scale unsaturated-zone flow model (Bodvarsson et al., 1997) and provided to the site-scale UZ flow and transport model (Robinson et al., 1996). Similarly, the source term for radionuclide transport in the unsaturated zone is provided by the calculated release from the engineered barrier system, $\dot{M}_i(t)$. Other parameters that are transferred between domains include the temperature (T), relative humidity (RH), number of corrosion pits in the waste package, liquid water saturation (S_l), chemical composition (C), radionuclide concentration (c_i), and mass release rates ($\dot{M}_i$) from other domains besides the EBS. Both the detailed and abstracted models corresponding to each box in Figure 7.2-1 are described in much greater detail in the various sections of Chapter 6. In so much as the form of the abstractions affects the code architecture, the abstractions are also discussed in abbreviated form in Section 7.2.2. (For example, the code architecture is different when it uses a response surface generated externally to RIP, read into a RIP cell environment, versus a dynamic call to an external process model while running RIP.)

7.2.1.2 Other Types of Abstractions Affecting TSPA-VA Model Architecture

If there were no computational resource or time limitations, one could run the detailed process models in the order shown in Figure 7.2-1 many (~100-1000) times, for each "discrete case", to develop a probabilistic distribution of overall repository performance [i.e., the final response of the farthest downstream model (the biosphere), which would include the combined effects of all models]. The 100-1000 realizations could be displayed as either a CDF or CCDF of peak dose that would represent parametric and conceptual-model uncertainty. In this context "discrete case" means that not all uncertainty will be subsumed into a single stochastic distribution of peak dose. For example, the backfill/no-backfill design option in the emplacement drifts would generally be represented as two discrete cases (two discrete CCDFs)—see Section 7.3.

For each discrete case, one would pre-generate 100-1000 realizations of the uncertain parameter values (e.g., solubilities, fracture/matrix interaction parameters, etc.) and then sequentially run each process-level model in its corresponding domain.[3] At the end of this procedure, the TSPA-VA would be complete, without the need for further abstractions, beyond the domain/process-based abstractions already discussed above. However, given the finite amount of computational time available, some further abstractions are usually required in order to run hundreds of realizations of the various subsystem models: (a) reduction to lower dimensionality, (b) coarser discretization of the spatial domain, i.e., fewer numerical grid blocks, and/or © reduction of the model to a response surface (or multidimensional table), which is a functional relationship between output (e.g., radionuclide concentration) versus key model parameters as a function of time.

<u>Dimensionality Abstractions</u>

As discussed in Chapter 6, dimensionality reduction is potentially being used in several areas, including far-field thermohydrology, far-field transport, near-field environment, and EBS transport. However, 3-D models are being used wherever feasible. The abstraction/testing analyses are using appropriate performance measures for each affected model to determine if the 2-D response will bound the more detailed 3-D model response at all $(\vec{x}, t)$ over the relevant domain.

<u>Response-Surface Abstractions</u>

Response surfaces represent the next level of abstraction following domain/process/dimensionality

[3] In general, there should be consistency of parameters across the model domains, e.g., matrix/fracture flow parameters in the UZ thermohydrology model should be the same as in the UZ transport model.

abstractions. They are usually represented as multidimensional tables, which require interpolation routines to determine responses in between the known table values. More generally they can be thought of as arbitrary surfaces on a graph in *n*-space. The main "abstraction" embodied in these functions is the interpolation feature: the fact that smooth functions are created from a set of discrete model calculations, and then linearity of the processes is assumed between the discrete points.

Response surfaces are feasible in the TSPA-VA model architecture because of the decoupling of domains and processes discussed above, which allows a number of the models to be run independently of each other. Response surfaces are desirable because the complexity of the detailed process models, resulting in lengthy computational times, makes it infeasible to couple all of these in the overall TSPA code and run them sequentially in real time in the order shown in Figure 7.2-1, for hundreds or thousands of realizations of the uncertain model input parameters. Rather, a number of these models must be run in parallel (i.e., simultaneously in real time) over perhaps tens (rather than hundreds) of realizations of the input parameters, in order to create output response surfaces for each model. These response surfaces are then used in the overall TSPA code, instead of the detailed models themselves.

There are a number of concerns with generating such response surfaces:

(1) If they are to be generated with the original 3-D models, computer time and resources may limit them to a sparse sampling of the key parameters. This could cause one to suspect the validity of linear interpolation between the sparse set of data points.

(2) When coupling (i.e., sampling) response surfaces over separate domains and process models, one must be certain to have common independent variables (parameters) amongst the response surfaces, for example, the response surfaces should be simultaneously sampled at the same value of the infiltration flux. This ensures self-consistency in the overall TSPA-VA model.

(3) Response surfaces from different domain/process-based models should be generated in a conceptually consistent fashion. For example, if a dual permeability model is used for UZ flow, then it should be coupled to a dual permeability model for UZ transport. Also, depending on the time duration of certain processes, it should probably also be coupled to a dual permeability model of UZ thermohydrology.

(4) Response surfaces are only valid if the independent variables account for almost all of the variability in the dependent variable. That is, if a response surface $z = f(x)$ is developed, and there is another variable y that affects z significantly, then the results could be inaccurate unless the response surface is expanded to be $z = f(x,y)$.

Temporal Abstractions

Point #3 in the previous section, regarding conceptual-model consistency, brings up yet another type of abstraction—temporal abstractions. As already shown in Chapter 6, these play an integral role in the TSPA-VA model architecture through the assumption of steady-state flow. Also, the use of the steady-state flow assumption for decoupling UZ flow and transport has already been discussed above in the context of process-based abstractions. Another example is related to the thermal decay pulse. In particular, it has been assumed in past TSPAs that the thermal pulse has fully decayed before radionuclides are released from the waste packages (or at least that the influence of the thermal pulse is minimal at that time). This allows different models and parameters to be used in the UZ thermohydrology model (e.g., equivalent continuum), which feeds the waste-package degradation model, compared to the UZ flow model (e.g., dual continuum). Thus, consistency becomes less of an issue. Even if the thermal decay pulse is still active at the time of waste package failure, it may still be possible to use different conceptual models for thermohydrology (equivalent continuum model—ECM) and UZ flow (dual permeability model—DKM), particularly if it can be shown that temperature predictions are about the same in both models. However, if flux predictions are very different, then some sort of analysis must be completed to show the applicability and/or conservative nature of the simpler ECM model. Nevertheless, an abstraction may still be employed in which one model is used during the time period of thermal perturbations and another model following thermal perturbations.

7.2.2 TSPA-VA Code Architecture

7.2.2.1 Overall Architecture

The overall model architecture and abstraction strategy for TSPA-VA discussed in the previous section forms the basis for the architecture of the overall TSPA-VA computer code. The executive driver program or integrating shell which links all the various models is RIP V5.x (Repository Integration Program, Golder, 1997).

RIP is a descriptive model rather than a process-based model, i.e., it generally represents in a simplified fashion what we already have determined from the more detailed models. However, the current version (5.x) has some very useful features such as cells and environments (described below), which allow certain processes to be modeled in reasonable detail. The RIP cells are basically equilibrium batch reactors and, by linking a number of these together, a fairly accurate description of the underlying processes can be realized. This will be the approach used for portions of the EBS part of the TSPA-VA analyses. RIP V5.x also has the flexibility to make external function calls to detailed process codes and coordinate the input/outputs amongst these programs and amongst the RIP cells. This will be the approach taken for the UZ and SZ domains. Also, response surfaces are generally input into RIP as "environments" for cells. They take the form of multi-dimensional tables.

The explanation of the TSPA-VA code architecture is divided into two sections that follow: the engineered barrier system (EBS), and geosphere/biosphere. As implemented in RIP, the EBS portion of the TSPA-VA code (waste-package, waste-form, near-field environment, and EBS transport) directly utilizes the cell or compartment model in RIP V5.x and therefore most (but not all) of this code is programmed directly in the RIP menus. On the other hand, the geosphere portion of the TSPA-VA code (unsaturated and saturated zones) are external function calls from RIP to more detailed process models (such as FEHM for the UZ). The biosphere portion is again contained in the RIP menus. [Although the EBS models are directly implemented in the RIP cells, they depend to a large extent on response surfaces generated by external process codes that were run prior to the full RIP runs, such as WAPDEG, which is a FORTRAN program that generates pit-growth and first-pit-penetration curves (Atkins and Lee, 1997).]

Finally, it should be noted that RIP V5.x forms the heart of the TSPA-VA code architecture because it is the probabilistic sampling program that ties all the other models/codes together in a coherent structure in order to conduct multi-realization runs of the various models to produce a final CCDF capturing uncertainty in all the models. Thus all models and response surfaces that are coupled to RIP must allow for consistent parameter sampling amongst themselves. For example, if a given infiltration rate is sampled at the beginning of a realization, this rate must be passed to all response surfaces and all external modules, in order to generate an internally consistent overall model of repository behavior. For example, that given infiltration rate will have a corresponding temperature and relative-humidity history produced by the NUFT thermohydrology model (Nitao, 1996), and a corresponding pitting history for the degradation of the packages as predicted by WAPDEG, and a corresponding set of chemical composition parameters as predicted by the near-field environment model, with respect to concrete liner degradation, package degradation, waste-form degradation, etc. Also, as discussed below, it will correspond to a pre-generated 3D flow field in the unsaturated zone.

7.2.2.2 Code Architecture for EBS Components

Figure 7.2-2 illustrates the planned model for the EBS portion of the TSPA-VA codes. In this diagram, boxes with double lines (cladding/waste-form, degraded package, and invert) are "associated" cells in RIP V5.x, i.e., their volume, area, flow rates, etc. are upscaled as a function of the number of failed packages. This upscaling is a byproduct of the abstraction which groups waste packages according to inventory and environment. In other words, it is not computationally efficient to model every distinct waste package (there are over 12,000 of them in the current design). Therefore, they are grouped or lumped according to their inventory and environment, which includes such factors as the temperature, relative humidity, and seepage flux, as well as the type and quantity of waste (whether commercial spent fuel, defense high-level waste, etc.) Typically, the 12,000 packages could be divided into anywhere from 20 to 200 distinct groups. As the packages within a given group fail, the RIP model lumps the failed packages into one "giant" package with the appropriate mass, area, and volume (Golder, 1997).

The three dashed-line boxes upstream of the waste form (i.e., the liner, dripshield/backfill, and degraded package) could also be represented as cells in RIP (though not as associated cells), but the TSPA-VA plan is to model these outside of RIP in process-level codes. For example, the concrete liner would be modeled in a geochemical reaction-path (EQ3/6—Wolery, 1992) and/or reaction-transport (AREST-CT—Chen et al., 1995) code, and the degraded package would be modeled in a corrosion code, such as WAPDEG. The chemical effects of a drip shield/backfill would also be modeled externally to RIP in a code such as EQ3/6 or AREST-CT. However, the primary function of a drip shield is to limit advective releases from the packages, and this function would be modeled directly within the RIP code.

The arrows in Figure 7.2-2 represent the input/output or response-surface connections between the various models/codes. The connections can be either one-way or two-way, e.g., the near-field environment model has two-way connections to all of the other models. Some of the other models, such as the concrete lining, though shown discretely in Figure 7.2-2, will actually be a part of the near-field environment model, rather than a separate model. The near-field environment code is likely to be a combination of several codes run for different scenarios, including the reaction path code EQ3/6, the reactive transport code AREST-CT, and the reactive transport codes OS3D/GIMRT (Steefel and Yabusaki, 1996).

Based on the schematic information transfer in Figure 7.2-2, it is clear that some response surfaces generated by codes external to RIP will just feed other codes external to RIP, e.g., chemical-composition response surfaces from the near-field model will directly feed the external model for waste-package degradation, WAPDEG. Other response surfaces, such as temperature, relative humidity, flux, and some compositional parameters will be fed directly into RIP as response surfaces (RIP "environments") that influence such things as the radionuclide solubilities, waste-form degradation rates, K_ds in the invert, etc.) The thermohydrology drift-scale code run external to RIP is planned to be NUFT (Nitao, 1996); however, at this stage it has not been determined if it will be run with the equivalent-continuum conceptual model (ECM) or the dual-permeability conceptual model (DKM). (More than likely, it will be either ECM or "generalized" ECM because of numerical difficulties with the DKM solution to the thermohydrologic equations for certain thermohydrologic property sets. Some limited sensitivity studies will be attempted to evaluate the impact, if any, of this modeling choice; but the success of these studies is dependent on being able to advance the DKM numerical models far enough in time to yield a valid comparison.)

Details of the EBS Source Term in RIP. As mentioned above, "cells" in the RIP code are batch reactors in a given spatial location. Our conceptual model for the RIP representation of the in-drift environment (including and downstream of the waste form) is to link several cells in series—with each cell representing a distinct physical-chemical environment, e.g., a "waste-form cell" connected to a "degraded waste-package cell" connected to an "invert cell". With respect to the downstream EBS environments (i.e., cells "associated" with the waste form), including the waste-form cell itself, it has tentatively been decided to divide each source term (i.e., each waste package) into several discrete spatial bins along the axis of the waste package. This discretization will be used primarily to account for drips on different parts of the package, and also for allowing these drips to move with time, encountering different portions of the waste-form with time. If, for example, a drip location remains steady in space for a very long time, this could imply that the waste form dissolves heterogeneously in space. For instance, if the dripping fracture were located at one end of the package, that end could completely dissolve by advective flow, but the remainder of the package could only interact with the drips by diffusive communication with the end of the package that encounters the drips. (It could also diffuse directly to the invert.)

For the purposes of the discussion in this section, and for illustrative purposes, we only show a division of the package into two sections. This is sufficient to illustrate the conceptual model outlined above. The model can be refined spatially if desired. Figure 7.2-3 is an illustration of the conceptual model of the downstream, "associated" EBS cells and shows a little more detail with respect to the source term than the previous figure. In particular, the fuel (waste-form) itself and the waste package are part of the source term in RIP, but are not modeled as cells per se. The mass released from the waste in the failed package ["primary container failure distribution" in RIP, which in our conceptual model includes both the inner corrosion-resistant material (CRM) and outer corrosion-allowance material (CAM) barriers] and the failed cladding ("secondary container failure distribution" in RIP, or possibly a modification to the fuel surface area) is released to only the first associated cells (i.e., the most "upstream" associated cells), which are designated in the drawing as "waste cell #1" and "waste cell #2". These two waste cells may be thought of as batch reactors containing water (and perhaps some solids, such as degraded basket and package materials) into which is dumped the dissolving waste based on the waste degradation rate, the solubilities, and the package failure distribution. If, for example, the solubility is quite low, the rate of mass input into the associated waste cells could actually be lower than the waste dissolution rate. (The other cells, such as the film cell and degraded package cells, receive mass after it has dissolved into the waste cells and been transported away from the waste cells via diffusion and/or advection.)

In the "drips on waste package" release model used in TSPA-1995 (M&O, 1995), release from a pitted package was via diffusion only, through corrosion products filling fully penetrating pits, i.e., the dripping advective flow of water could not directly contact the waste form itself.[4] In Figure 7.2-3, this diffusive release model will probably be implemented as a changing diffusion area in the connection between the fuel cells and the film cells and between the fuel cells and the degraded WP cells beneath the package. (The diffusive area would have to be apportioned appropriately between the film cell and the degraded package cell. Perhaps the film cell will be thought to completely surround the package and then all the diffusive area would be assigned to the film cell.) Another point is that although the degraded package is shown in Figure 7.2-3 as a single RIP cell, in reality it will likely be several RIP cells. This additional degree of discretization will be necessary in order to adequately represent the concentration gradient (and thereby the diffusive flux) across the degraded package materials.

Finally, the invert cell in Figure 7.2-3 will be given the hydrologic and chemical properties of (degraded) concrete for the TSPA-VA base case. For packages that have no advective releases (i.e., no dripping water), but only diffusive releases, these properties can have a strong effect on the mass transfer rate of radionuclides out of the drift environment and into the geosphere. For example, if capillary equilibrium is established between the invert and the surrounding host rock, then the water saturation of the invert material will be at residual saturation, and if this is low, the diffusion rate could be quite low (Conca and Wright, 1992). The saturation time history for the invert cell will be

[4] We intend to have a time-dependent EBS model which shifts at late time from diffusion through the waste package ("drips on waste-package" release model) to advection (dripping) through the waste package ("drips on waste-form" release model) to account for degradation of the inner and outer waste-package barriers.

determined external to RIP in the NUFT thermohydrology code and then fed into RIP as a response surface.

7.2.2.3 Code Architecture for Geosphere Components

Figure 7.2-4 is a schematic of the code architecture for the entire TSPA-VA; it is Figure 7.2-2 with the geosphere/biosphere components added. The two dotted boxes in Figure 7.2-4, i.e., the unsaturated zone and saturated zone, could be modeled as a series of cells within RIP; however, the plan is to model them as external function calls. For the unsaturated zone flow and transport, the intent is to directly call the 3D site-scale transport model (Robinson et al., 1996) as implemented with the FEHM particle tracker module (LANL, 1997). Thus, during a given realization, for every simulation time step in RIP (e.g., 100 years) source term information (specifically, radionuclide mass fluxes) will be passed from the RIP EBS cells to the FEHM particle tracker, which will then move the particles as far as they would travel during that time step. FEHM will also pass back to RIP the mass flux that leaves the UZ model domain in FEHM, i.e., the mass to be passed to the saturated-zone model. FEHM will not calculate the flow field dynamically, only the transport. The flow fields are intended to be pre-generated with TOUGH2 (Pruess, 1990)—which implies the assumption of steady state flow—and there will be a library of flow fields corresponding to the uncertainty in the UZ flow parameters and infiltration rate. For each realization, a different flow field will be sampled based on a sampling of the key uncertain parameters responsible for that flow field. In addition, the response surfaces from the other TSPA-VA models, such as thermohydrology, near-field environment, etc., will have to be sampled with the same parameter set that corresponds to that flow field.

The SZ model will be connected similarly, i.e., it will be an external function, to which RIP will pass the output mass from the UZ FEHM particle tracker. In turn, the SZ output parameters (concentration and flux at a given location) will be passed by RIP to the biosphere model. The dispersion model in the FEHM particle tracker does not specifically model longitudinal and transverse dispersion,[5] and is thus not appropriate for modeling SZ transport, for which dispersive processes are expected to play a much more important role compared to UZ transport—because of the much longer transport distances.[6] However, calling the 3D FEHM finite-element model for each RIP realization requires too much computational time, therefore, an abstraction will be made. The plan is to assume steady state flow and then use linear convolution. In particular, a unit-pulse source term will be applied over the footprint of the repository at the water table and the breakthrough curve of this mass at some distance downgradient in the SZ (likely at 20 km) will be calculated. This breakthrough curve will be computed for the full 3D SZ flow and transport model over a range of

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[5] The FEHM particle tracker has dispersion in the x, y, z directions in the global (but not local) coordinate system. For UZ transport (which is predominantly vertical, and of much shorter distance than SZ transport), this model of dispersion is felt to be sufficient.

[6] Diffusive processes (particularly between the matrix and fracture media) are also expected to be quite significant in the SZ based on recent well-to-well tracer tests at the C-Holes Complex (Reimus and Turin, 1997).

the key parameters. This will be accomplished with the finite-element solution of the flow and transport equations in FEHM. This will provide a library of breakthrough curves over a range of key parameters. Then, once the actual source term at the water table is determined by running all the models upstream of the SZ (for each stochastic realization), this source term can be convolved with the pre-generated SZ breakthrough curves to determine the actual breakthrough curve with a time-varying source term. This method has been described by Robinson et al. (1997). The key to the applicability of this method is whether the linearity assumption is justified for all the important radionuclides and whether the flow field is steady. This will depend in large part on how much climate change influences the saturated zone. (Treating radionuclide chain decay and daughter production also requires special treatment with the convolution method, however, for the most important radionuclides from a performance perspective, radioactive decay and production is not expected to be so important on the time scale of transport through the saturated zone.)

If the convolution method proves to be unworkable, then the next best method would be to try to simulate a 2D vertical cross-section[7] along the centerline of the main contaminant plume using FEHM and calling this from RIP. If this is not feasible, then we may have to go back to a simple 1D model, or a "bundle" of 1D tubes, as used in TSPA-1995 (M&O, 1995) and TSPA-1993 (Wilson et al., 1994). This method could also be implemented within RIP, using the RIP cells or pipes algorithms (Golder, 1997).

The biosphere will be modeled within RIP as a cell connected to the radionuclide mass concentration and flux output from the SZ model, but with biosphere dose conversion factors (BDCFs) computed by models outside of RIP and input as tables. (Each BDCF will be input as a probability distribution—see Section 6.9.)

A final note on the geosphere models/codes is the climate model. In order to implement decoupled flow and transport models (i.e., in order to use the steady state assumption), climate change will be implemented as a series of step changes, which instantaneously change the flow field in the UZ and SZ. (It may also change the water table height in the SZ.) When sampling the climate change model within RIP, this requires coordination amongst the coupled geosphere submodels in that they must all simultaneously change to the appropriate climate state. Practically speaking, the steady-state flow fields corresponding to different climate states (i.e., different infiltration rates) will be pre-generated with TOUGH2. Then, according to the particular time history of climate changes sampled by the RIP TSPA model at the beginning of a given realization, the UZ flow field library will have to be interrogated for a different flow field at every time during the simulation when a step change is indicated. This change in a flow field will be assumed to apply instantaneously to the transport model. The validity of the step-change sequence of climate changes versus a transient flow model

[7] A 2D vertical cross-section is expected to be more representative than a 2D horizontal cross-section because of the shape of the source term. The UZ source term is much, much wider than it is thick (it just drops mass into the very top of the SZ over a width of perhaps 4 km perpendicular to the general SZ flow direction). Thus, transverse dispersion in the vertical direction should have a much greater effect on the concentration peak than horizontal transverse dispersion.

is being investigated in some of the abstraction/testing plans (e.g., M&O, 1997). As concerns the effect of climate change on the thermohydrology model, the plan is *not* to generate a set of different temperature (T) and relative humidity (RH) responses for different steady state flow fields, but to generate T and RH responses that are a product of a time-varying infiltration boundary condition. Thus the paradigm for climate change as implemented in some of the near-field models (e.g., the waste-package degradation model) is slightly different than the far-field models. In particular, the waste-package degradation model will have as input the T and RH responses from the thermohydrology model that are a function of a time varying infiltration boundary condition, whereas the transport model will have a series of steady state flow fields that are a function of constant boundary conditions but that are pieced together later, with the assumption that the transient effects during the change from one climate state to the next are minimal.

7.2.3 TSPA-VA Software Quality Assurance: Configuration Management and Verification

Several software codes will be used in the development of TSPA-VA. At the time of this document, the codes are RIP, FEHM, TOUGH2, WAPDEG, AREST-CT, EQ3/6, and NUFT. The codes are in various levels of QA configuration. The status and objectives for configuration management and verification of the codes is described in this section.

The RIP code is acquired software developed by Golder Associates. RIP is developed, tested and maintained in accordance with *Golder Associates Quality Management Plan for Seattle Operations*, an ASME NQA-1-1994 compliant quality assurance program. Golder Associates implements an automated software configuration management program based on PVCS Version Manager and PVCS Tracker by Intersolv, Inc. The Golder Associates Software Configuration Management system includes mechanisms for revision control and change tracking. The Change Tracking system manages problem reports and change requests associated with the RIP code.

Golder Associates verifies each new version of RIP via a rigorous suite of verification tests before the version is released. The current RIP verification plan includes approximately 500 individual tests that exercise various combinations of features implemented in RIP. The verification test results are compared to known analytical or numerical solutions (Golder, 1997).

The M&O plans to treat RIP as acquired software and bring it under the M&O Software Configuration Management System in accordance with M&O Quality Administrative Procedures QAP-SI-0 Computer Software Qualification and QAP-SI-3 Software Configuration Management. M&O control of RIP will include process controls for installation, and preparation of a Software Qualification Report.

The Finite Element Heat and Mass transfer code (FEHM) was developed for use at Yucca Mountain by Los Alamos National Laboratory. FEHM was verified through rigorous and complete testing of the model, using known analytical solutions or, in the case where an analytical solution does not exist, the code was benchmarked against the results of other similar numerical models. There were a number of test cases and comparisons performed to verify the use of FEHMN, including tests of thermodynamic functions, 2-D and 3-D heat conduction, heat and mass transfer, and fracture transport/matrix diffusion. Additionally, FEHMN results were compared to National Bureau of Standards Steam Table data and TOUGH2 results (Dash, et al, 1995).

The approach in TSPA-VA to dynamically link FEHM to RIP requires special treatment to ensure traceability and integrity of data transfer between the two codes. RIP V5.x can call FEHM as a Dynamically Linked Library (DLL) file, thus eliminating the need to modify any of the RIP or FEHM algorithms. Simple data-passing tests will be performed to confirm that parameters are being correctly passed between the two codes.

The TOUGH2 code (Pruess, 1990) is acquired software that was initially developed by Lawrence Berkeley National Laboratory and has been modified by Sandia National Labs. TOUGH2 is a multi-dimensional numerical code used for simulating the transport of water, vapor, air, and heat in porous media. Each TOUGH2 modification performed by SNL is systematically proposed and verified through a verification plan and validation report, as prescribed by SNL QAIP 19-1, Software Quality Assurance Requirements, before it is released.

The WAste Package DEGradation (WAPDEG) code is software developed for the Yucca Mountain Project by the M&O Performance Assessment Organization. The WAPDEG code is used to simulate waste package degradation and will be further developed and tested in accordance with M&O Quality Administrative Procedure QAP-SI-0 Computer Software Qualification. Configuration management of the software will be controlled by M&O QAP-SI-3 Software Configuration Management.

The Analyzer of RadionuclidE Source-Term with Chemical Transport (AREST-CT) is a scientific computer code designed for reactive transport simulations, and is being used for performance assessment of the geochemistry of the engineered barrier system. The AREST-CT code has the capability to analyze the degradation and release of radionuclides from the waste form, chemical reactions that depend on time and space, and transport of the waste and other products through the EBS. Version 1.0 of AREST-CT was developed at Pacific Northwest National Laboratories (Chen et.al, 1995). AREST-CT is currently being modified and updated by the M&O Performance Assessment organization. The M&O currently plans to treat AREST-CT as developed software. The M&O plans to bring AREST-CT into the M&O Software Configuration Management system in accordance with M&O Quality Administrative Procedures QAP-SI-0 Computer Software Qualification and QAP-SI-3 Software Configuration Management. M&O control of AREST-CT will include process controls for installation, and preparation of a Software Qualification Report.

EQ3/6 is a computer program for reaction-path modeling of geochemical systems developed by Lawrence Livermore National Laboratory. Software quality assurance for EQ3/6 is carried out in accordance with the Individual Software Plan required by Lawrence Livermore National Laboratory Quality Procedure 033-YMP-QP 3.2 Software Quality Assurance. The EQ3/6 Software Test and Verification Report describes the test and verification cases to qualify the code (Kishi, 1996). The M&O plans to bring EQ3/6 into the M&O Software Configuration Management system in accordance with M&O Quality Administrative Procedure QAP-SI-3 Software Configuration Management.

NUFT (Nonisothermal Unsaturated - Saturated Flow and Transport model) is a suite of multiphase, multicomponent models for numerical solution of non-isothermal flow and transport in porous media (Nitao, 1996). Software quality assurance for NUFT will be carried out in accordance with the Individual Software Plan required by Lawrence Livermore National Laboratory Quality Procedure 033-YMP-QP 3.2 Software Quality Assurance. The first stage of the code verification for NUFT using one-dimensional problems has been completed (Lee et al., 1993). Additionally, NUFT has been benchmarked against the V-TOUGH code for a wide range of problems related to decay-heat-altered nonisothermal flow and transport at Yucca Mountain (Wilder, 1996).

MCNP (M&O, 1997b) is a general purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems. The MCNP code package was developed by Los Alamos National Laboratory. MCNP has been validated for use in quality affecting applications (criticality safety) by the M&O in accordance with the M&O Quality Assurance Procedures. The validation is documented in the Software Qualification Report for MCNP4A, CSCI: 30006 V4A.

GENII is a system of seven computer codes used for estimating potential radiation doses to humans as a result of radionuclides in the environment. The codes address both routine and accidental releases of radionuclides to air or water. Internal radiation dose calculations are performed using the methods recommended by the International Commission on Radiological Protection. The codes were originally developed in accordance with the Pacific Northwest National Laboratory Quality Assurance Program. (Napier, et al. 1988) The M&O plans to treat GENII as acquired software and bring it under the M&O Software Configuration Management System in accordance with M&O Quality Assurance Procedures. M&O control of GENII will include process controls for installation, and preparation of an Software Qualification Report.

The Microbial Impacts to the Near-Field Environment Geochemistry (MING) code is under development by the CRWMS M&O. The MING code will be used to estimate the impacts of microbes to the near field environment geochemistry. The program takes into account the availability of nutrients and the energy necessary to convert those nutrients to microbes, the level of oxygen in the repository, as well as the moisture content of the repository atmosphere. Materials identified in the repository design are decomposed into their basic elements over time and their contributions to the life of the microbes is included in the ground water passing through the repository. MING will be developed and tested in accordance with M&O Quality Administrative Procedure QAP-SI-0 Computer Software Qualification. Configuration management of the software will be controlled by M&O QAP-SI-3 Software Configuration Management.

Configuration Management.

TSPA-VA will use a number of computer codes to simulate the relevant features of the Yucca Mountain repository. All of the codes that are used to support TSPA-VA will be placed under the controls of a configuration management program. The software configuration management program is documented in M&O procedure QAP-SI-III "Software Configuration Management." The software configuration management program include software configuration identification, configuration control, and configuration status accounting.

Configuration Identification

Software configuration identification, including version or revision, is provided through the use of a unique CSCI identifier that is assigned to each individual software product. A series of Document Identifiers (DIs) and Media Identifiers (MIs) relate these baseline elements to the associated software CSCI product and enables cross-referencing of the individual baseline elements.

Configuration Control

Configuration control provides the structure for establishing new software baselines, software routines, releasing software baselines to users, and receiving those evaluated and approved changes from the Responsible Manager, including withdrawal and retirement to existing software baselines. Configuration control includes establishing baselines, proposed changes to existing baselines, retirement, and impact assessments of supplier-provided (if applicable) error reports from the Responsible Manager.

Configuration Status Accounting

Configuration status accounting is implemented through the software configuration status accounting system. Information contained in the status accounting system provides reports on approved baseline elements, identifiers, proposed and approved changes, and brief descriptions of changes made between versions of software configuration items.

7.3 TREATMENT OF UNCERTAINTY AND VARIABILITY

7.3.1 Introduction

Uncertainty means not having sure knowledge. Variability means having variation in time or space. Here we use the term uncertainty to describe features, events, or processes (FEPs) with doubtful outcomes or properties that cannot be predicted *a priori*. We use the term variability to describe FEPs that are known to exist or occur, but that can take on different values in different regions of the spatial-temporal domain. In general, variability can serve to disperse and dilute contamination from a repository in either time or space. Uncertainty, however, can only cause, at best, confusion and, at worst, error. Uncertainty and variability are related, in that the spatial and temporal variability are generally quite uncertain.

In TSPA, we use two basic tools to deal with uncertainty and variability: (1) alternative conceptual models and (2) probability theory. Uncertain processes often require different conceptual models. For example, different concepts of matrix/fracture coupling in the unsaturated zone lead to different flow and transport models. Sometimes, conceptual models are not mutually exclusive (e.g., both matrix and fracture flow might occur); sometimes they do not exhaustively cover all possibilities (although matrix and fracture flow apparently do). These problems indicate that use of alternative conceptual models is not rigorous, an unfortunate characteristic of uncertainty. Alternative conceptual models can either be analyzed with side calculations or within the TSPA calculations themselves (see Section 7.4).

Probability distributions are used to describe uncertain parameters. In a TSPA calculation, the distribution is sampled for a specific value to be used in one realization of a Monte Carlo simulation. Other realizations use other sampled values. (The solution to a realization defines one point in the solution space; many realizations define a subset of the solution space from which a probability distribution can be approximated.) Spatial variability can be either defined by a function (perhaps with some uncertain parameters as part of the functional definition) or randomly, depending on which is more appropriate for a particular variable. Spatially variable rock properties (e.g., permeability) can also be defined by use of geostatistics. In this case, a probability distribution is sampled and a representation of the physical domain is constructed before the TSPA simulation. The TSPA realizations are then solved using these domains.

The Monte Carlo method has been used in all TSPAs to date and it will be the primary method of uncertainty analysis used for TSPA-VA. It involves calculating numerous "realizations" of the repository system. Each realization has an associated probability, so that there is some perspective on how likely or unlikely that set of circumstances is. (In the standard Monte Carlo method, each realization is equally likely, so the probability is just one divided by the number of realizations. In more elaborate variants, for example using "importance sampling," some realizations can be less probable than others.)

The Monte Carlo method produces a range of calculated performance measures (e.g., dose to a reasonably maximally exposed individual within a given time period in a given location) together with a probability for each one. In a manner of speaking, it gives an estimate of repository performance plus "error bars" on the estimate. The performance measures and probabilities have traditionally been presented in the form of the complementary cumulative distribution function, or CCDF, because it shows at a glance the probability of exceeding a given performance-measure value.

7.3.2 Weighting of Alternative Conceptual Models

In many subsystems of the overall TSPA system, there are plausible alternative models or assumptions. In some cases, these alternatives form a continuum, and sampling from the continuum of assumptions fits naturally within the Monte Carlo framework of sampling from probability distributions. In other cases, the assumptions or models are discrete choices. In particular, various processes (such as fracture/matrix interaction, infiltration, cathodic protection, galvanic proteetion, drift seepage, diffusive versus advective release from waste packages, etc.) are so highly uncertain that instead of developing meaningful continuous probability distributions over the postulated parameter ranges, discrete distributions have been proposed in past TSPAs consisting of only a few parameter values (often with equal weighting). Alternatively, different conceptual models of a given process are postulated (again, frequently with equal weighting), based on different sets of physical-chemical parameters. Discrete sets of assumptions, discrete models, or discrete parameter distributions can be sampled in a Monte Carlo simulation (the probability distribution is a set of discrete points or delta functions rather than a continuous function), but sometimes it seems artificial to do so, or it is hard to justify weights (probabilities) for the discrete cases. There are thus two possible approaches to incorporating discrete alternative models within the TSPA: by rolling everything together into one comprehensive Monte Carlo simulation, or by keeping the discrete cases separate and performing multiple Monte Carlo simulations with various combinations of the assumptions. The latter approach was used for TSPA-1995 (M&O, 1995).

There are advantages and disadvantages to both approaches. Let us refer to them as "lumping" and "splitting," respectively. Lumping has the conceptual advantage that a single CCDF is generated that can be said to include all the system uncertainty. Splitting can easily lead to a confusing profusion of cases, and it can be difficult to quantify the relative importance of the various discrete assumptions. If there are many discrete cases, splitting probably requires more work (i.e., more calculations of the total system) as well. For example, if 100-realization Monte Carlo simulations were conducted for each of these discrete cases, it could require an enormous number of combinations to cover the entire sample space ($n_1 \cdot n_2 \cdot n_3$.....), where n_i is the number of discrete values for the *i*th model/parameter. Also, the individual CCDFs that are presented for each of these cases would not be representative of the overall uncertainty in the system, since most of that is contained in the various discrete distributions. (The remaining uncertainty in the discrete-case CCDFs would only be due to those few parameters that were assigned continuous probability distributions *a priori*.). The main disadvantage of lumping is the concern that cases with poor performance might be "diluted" within a sea of more favorable cases. That is, there could be a combination of the discrete assumptions that has poor performance, which might not be obvious under the lumped approach but which would stand out if that combination were presented separately. The other potential disadvantage of lumping occurs if there is no good justification for the probabilities used; if the weighting of the alternatives is artificial, then the results will be artificial as well.

For TSPA-VA, a combination of the two approaches will be used. If possible, we would like to generate a CCDF representing all the uncertainties of the whole system. Thus, to the extent possible, equally weighted alternative conceptual models (and also uniform parameter distributions) will be minimized *a priori*, based on available data and expert judgement. Based on the resulting weighted distributions, a CCDF of peak dose may be created that represents nearly all uncertainty and variability in the total TSPA and subsystem models. This "lumping" method of combining alternative conceptual models into one CCDF could take as much computational effort as the first "splitting" method of generating all combinations (but not weighting them), however, it does provide the potential for fewer realizations. The overall "lumped" CCDF method does require quite a few combinations of the various process models and abstracted models in order to develop a meaningful overall CCDF, i.e., one that is not too sparsely populated with data. However, with Latin Hypercube Sampling (LHS) it is expected that considerably fewer combinations from the discrete distributions are needed than the entire sample space—which would seemingly be the requirement for the equally-weighted "splitting" procedure described first.

This lumping approach clearly works best if the number of discrete unweighted sets of assumptions is minimized *a priori*. There may be a few discrete assumptions that just cannot reasonably be handled this way, which could lead to a (hopefully) small number of discrete cases. A possible example would be the alternative ECM and weeps models for UZ flow that were treated in TSPA-1993 (although the current plan for TSPA-VA is to create a continuous distribution of flow models between these two end-members). Also, for alternative repository designs, such as point thermal loading versus line thermal loading, it is clearly necessary to show different overall CCDFs, since there is no reasonable conceptual justification for lumping together these *a priori* design options. Furthermore, the main reason for displaying different CCDFs for different designs is to help choose the most beneficial design.

Because there will also be questions arising regarding the actual weights assigned to alternative conceptual models, we will present not only the overall lumped CCDF, but will in addition "take apart" the overall lumped CCDF by selecting the realizations corresponding to different discrete models and/or sets of assumptions, and then presenting these subsets of results separately for comparison (these are, in effect, conditional CCDFs). This will allow reviewers/regulators to choose the "most conservative" conditional CCDFs, if desired.

7.3.3 TSPA-VA Base-Case

As first mentioned in Section 5.1, the language of the 1997 Energy and Water Appropriations Act defines the overall scope and objectives of TSPA-VA:

> "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"

This "probable" behavior of the repository is intended to be represented by the TSPA-VA "base-case" models described in Sections 6.x.6 in the previous chapter. These models are summarized in Table 7.3-1. As described in Chapter 6, the base-case parameter sets and conceptual models for all the various component models in TSPA-VA generally encompass a *range* of uncertainty for the various parameters, rather than just one realization of the parameters. Thus, based on a random Monte Carlo sampling of the probability distributions for these parameter ranges, a base-case probability distribution (usually presented as a CCDF) of the repository behavior can be created. However, in light of the discussion in the previous section, this will be a conditional "base-case" CCDF, representing only one of the several possibilities from the various alternative conceptual models. In particular, as described in each of the Sections 6.x.6 in the previous chapter, the distinction between the "base-case" and the "sensitivity cases" was based on two criteria: (1) alternative conceptual models and (2) alternative designs. Thus, by implication, the "base-case" TSPA-VA model and corresponding CCDF represents the current best judgement as to the expected (or mean) CCDF of repository behavior (for a given design), without yet assigning this behavior an exact probability within the overall framework of the base case combined with the sensitivity cases.[8] This implies that the TSPA-VA "base-case" will not be the overall "lumped" CCDF described in the previous section. Furthermore, at this writing, the weighting of some of the alternative conceptual models is a work in progress. Thus, the final overall distribution (CCDF) of repository behavior, and the corresponding single expected-value (or mean-value) realization from this distribution (described below), will only be produced after the combined base-case and sensitivity-case models/simulations are completed.

In addition to specifying a "base-case" CCDF, as described above, which is a useful way of separating the most uncertain parameters/models from those thought to be better known, one should also specify an actual "base-case" time history of the repository behavior. This would be the single realization of all parameters that best represents the "probable" future performance of the repository. Normally, this would be chosen as the model/parameter realization that falls nearest the arithmetic mean of either the base-case conditional CCDF or the overall lumped CCDF (representing base-case plus sensitivity cases). The definition of this expected-value or mean performance clearly depends on the specific performance measure used. For example, the 1,000,000-year peak-dose mean behavior may be derived from a considerably different realization of the model parameters than the 10,000-year peak-dose expected-value case.

A dose time history will be displayed for the mean realization, as will the time histories of key outputs from the subsystem or component models—see Section 7.4. This time history will not necessarily be the same behavior that would result from just taking the mean, μ, of all individual distributions. Also, for both the base-case CCDF and the overall CCDF, the $\mu\pm1\sigma$ and $\mu\pm2\sigma$ time histories (i.e., the combinations of models/parameters that fall nearest the $\mu\pm1\sigma$ and $\mu\pm2\sigma$ points on the CCDF) will be presented (where σ is the standard deviation of the distribution).[9]

One potential problem with choosing the μ point from the base-case or overall CCDF and displaying its time history as the probable repository behavior, is the fact that the overall CCDF is based on only one data point (i.e., the peak dose) out of the entire time history for each realization. Since the

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[8] After completing the analyses for both the pre-defined base case and the sensitivity cases, the "base case" parameter ranges may be redefined based on the new knowledge, i.e., redefined to be closer to the mean CCDF of the total sample space of CCDFs generated from the sensitivity cases.

[9] The median or 50th percentile time history may also be presented as a useful estimator of future repository behavior.

overall CCDF may be generated from coarsely discretized parameter distributions, and is populated somewhat sparsely with data points, this could imply that the mean (μ) time history could be somewhat different than the ($\mu + \delta$) time history (where δ is a very small number), since it could represent quite a different combination of models/parameters than the μ time history. The same precaution would apply to the $\mu \pm 1\sigma$ and $\mu \pm 2\sigma$ cases. However, given that peak dose is expected to be the regulatory measure of concern, this issue may not be all that important. Besides, as part of the results, the effect of the most important parameters on the final CCDF will be shown explicitly using some method of uncertainty importance analysis (see Section 7.4).

7.3.4 Uncertainty and Variability in Each TSPA-VA Component Model

Below we discuss how uncertainty and variability in each component of TSPA-VA is to be included in the analyses and results. The particular types of uncertainty and variability discussed (see Table 5-1) typically correspond to the most important performance-affecting issues related to these components. (See respective subsections in Chapter 6 for a more complete description for each component and Section 5.4 for a general discussion of the various types of uncertainty to be included in TSPA-VA.)

7.3.4.1 UZ Flow

The basic strategy for TSPA-VA is to construct a set of 3-D UZ-flow realizations that are all calibrated to matrix saturations, perched water, and other available UZ data. Large-scale spatial variability will be an intrinsic part of each realization. Temporal variability caused by climate changes will be included by means of a series of steady-state flow fields. The set of flow realizations (10 or more) will include different infiltrations, matrix/fracture couplings, hydrologic properties, and climate-change assumptions in order to determine the impact of uncertainties in those parameters. In conjunction with UZ thermohydrology, a model for seepage into emplacement drifts will be developed that includes uncertainty and spatial and temporal variability by means of a link to the computed UZ-flow field as well as additional probabilistic considerations in determining the distribution of seepage rates and how many waste packages may be contacted by seepage.

7.3.4.2 UZ Thermohydrology

The basic strategy for TSPA-VA is to calculate drift and waste-package parameters (temperature, relative humidity, air mass fraction, gas-phase flow rate, liquid saturation) prior to the Monte Carlo simulations, then use table look-ups during the actual simulations. Temperature, relative humidity, and liquid saturation will be calculated with a multi-waste-package 3-D drift-scale model. The other quantities will be calculated with a 2-D mountain-scale model. The drift-scale model includes eight waste packages in order to capture variability in waste-package thermal output. Near-field spatial variability will be included (temperatures, etc., at multiple locations around multiple waste packages), and in addition larger scale spatial variability will be included by repeating the drift-scale calculations for multiple repository locations (at a minimum, "center" and "edge" locations). TSPA-VA will incorporate thermal effects on UZ radionuclide transport as a perturbation to the

UZ-flow velocities. The perturbation will be applied in the form of multipliers calculated for various locations using the mountain-scale model. Seepage into drifts is discussed above under UZ flow. Thermohydrology effects will be taken into account during the thermal period.

Uncertainty will be included in the UZ-thermohydrology modeling by considering multiple assumptions about initial infiltration, climate-change infiltrations, and possibly hydrologic properties and occurrence of rockfall.

7.3.4.3 Near-Field Geochemical Environment

Geochemical parameters important to waste-package and waste-form degradation, as well as EBS and UZ transport, will be uncertain and variable. Although it is desirable to describe these with continuous probability distributions, the amount of computational time and analysis effort required necessitates that the geochemical uncertainty and variability be described with discrete distributions representing discrete spatial locations and discrete scenarios (see Section 6.3). Thus, distributions of pH, Eh, chloride and fluoride concentrations, etc. will be calculated beforehand and placed in tables (response surfaces), and indexed by time and location for retrieval during the TSPA calculations. Spatial variability will be included in that multiple locations will be defined. Uncertainty will be included by producing ranges of chemical parameters (e. G., pH, etc.) that can be sampled from.

7.3.4.4 Waste-Package and Drip-Shield Degradation

Waste-package degradation depends on temperature, relative humidity, presence of seeping water, and rate and chemistry of the water if there is seepage. These items all have uncertainties and variabilities that are discussed above. In addition, there are uncertainties in the corrosion rates, presence and significance of microbial influence, effect of heterogeneities such as welds, effects of rockfall, and number of juvenile failures.

Waste-package degradation will be calculated with a model external to RIP and tables will be created that give the fraction of failed waste packages in a group and the number and sizes of openings in failed waste packages as a function of time and location (for several representative repository locations). The model calculations will consider corrosion rates, microbial activity, and the location of dripping water probabilistically. Response surfaces of degradation rate (first pit breakthrough and pit growth rate) will be created as a function of these various processes and other environmental parameters; the TSPA calculations will sample from the response surfaces. Damage from rockfall and the number of juvenile failures will be sampled from distributions.

Degradation of drip shields is just now being investigated, but likely mechanisms (e.g., earthquakes) are uncertain and variable and will probably be described with informed, but assumed probability distributions.

7.3.4.5 Waste-Form Degradation

Calculations for TSPA-VA will model waste-form degradation as a rate; the rate will be in the form of a distribution that will be sampled initially for each container group, combined with functional dependence on temperature, water chemistry, and seepage flux if likely. For spent fuel, the rate will be constrained by the fraction of fuel exposed by failed cladding. A cladding-degradation model is presently being developed that should incorporate a number of probabilistically defined parameters and functional dependence on temperature and water chemistry. The model will output a table giving the fuel exposed as a function of time; the table entries might be distributions to be sampled during the TSPA calculations.

7.3.4.6 EBS Transport

The EBS-transport component of TSPA-VA has two main parts: solubilities and transport mechanisms. Solubilities regulate the quantity of radionuclides that can be transported, and will be (at least for key radionuclides) functions of chemistry and temperature. This implies spatial and temporal variability because of the variability of the chemistry and temperature, discussed above. Solubilities are also fairly uncertain, and so either solubilities or parameters that determine solubilities will be sampled from distributions. Solubilities will be most important for slightly sorbing radionuclides, such as ^{237}Np, based on past TSPAs. For nonsorbing radionuclides with high average solubilities, such as ^{99}Tc and ^{129}I, the uncertainty and variability in the solubility parameter distributions is of little consequence, since their release rate from the EBS will be dissolution-rate-limited.

The EBS radionuclide transport depends on whether there is seepage present, on the rate of seepage if there is, on liquid saturation, and on size and number of waste-package penetrations. Those quantities all have associated uncertainties and variabilities, discussed above. There might be additional uncertainties introduced in the EBS-transport model, such as the probability that dripping water occurs at a waste-package opening, water-film thickness, a distribution for hydrologic properties of materials filling waste-package openings, or a tortuosity factor for transport inside the waste package, but these details have not been decided upon.

7.3.4.7 UZ Radionuclide Transport

UZ radionuclide transport will be calculated by a particle-tracking method, using the 3-D UZ-flow fields as modified by thermohydrology during the thermal period. Thus, all of the uncertainty and variability listed above for UZ flow applies also to UZ transport. In addition, we will consider uncertainty in radionuclide sorption coefficients, and possibly dispersivity and matrix diffusion, by sampling them from distributions.

One important uncertainty—the significance of colloid-facilitated transport—is being addressed by a sensitivity study to determine whether some form of colloid transport should be included in the main TSPA calculations.

7.3.4.8 SZ Flow and Transport

For TSPA-VA, saturated-zone radionuclide transport will be based on a set of calibrated 3-D site-scale flow models, which include large-scale spatial variability of hydrologic properties.–Each flow model will describe a different conceptual model of the structure of the SZ. One or more flow models might be constructed with different permeability values. Flow models will also be constructed for several different climates. The transport models will also be in 3-D and will generate breakthough curves for radionuclides at 20 km down-gradient from a repository. Several transport calculations might be performed for each flow calculation to look at uncertainty; the transport calculations might look at different K_d's, dispersivities, or rates of matrix diffusion. Convolution integrals will be developed for each of the transport models. The TSPA-VA calculations use the convolution integrals to determine, at each time step, the concentration of a radionuclide at 20 km from a given input under the repository.

7.3.4.9 Biosphere

Biosphere will be modeled within TSPA calculations through Biosphere Dose Conversion Factors (BDCFs). A separate BDCF will be developed for each radionuclide, but each BDCF will contain the doses for all pathways for each major scenario. The BDCFs will be calculated probabilistically and each will be a probability distribution. During a TSPA realization, radionuclide concentrations will be calculated at each time step at the geosphere/biosphere interface, BDCFs for each radionuclide will be sampled, the concentrations and the applicable BDCFs will be multiplied, and the products will be summed to represent the dose.

Calculation of BDCFs will consider uncertainty by using probability distributions for appropriate parameters. For example, plant uptake and soil buildup of radionuclides will be described with probability distributions. Human behaviors change over time in response to environmental changes and fashion, and these changes present an potentially insurmountable uncertainty. The strategy for TSPA-VA is to base human demography [foods consumed, time spent outdoors, hobbies (e.g., gardening), occupations (e.g., animal husbandry), etc.] on data from a survey of the existing population.

Spatial variability will be examined by calculating doses to a reference person located at different distances from the repository (5 km, 20 km, 30 km, though 5 km and 30 km may be included only as sensitivity studies). In addition, some spatial variability is implicit in the parameter probability distributions.

TSPA-VA calculations for disruptive events might handle the biosphere differently, with simplified calculations to look at dose from specific pathways (e.g., inhalation of volcanic ash).

7.3.4.10 Disruptive Scenarios

Seismicity causing rockfall is the only disruptive event that is expected to occur with certainty and will be included in all TSPA-VA calculations (except those with backfill). Timing of rockfall will be sampled from recurrence times of major earthquakes; amount of and location of rockfall will be random. (Rockfall will also be tied to thermal effects.) Other seismic effects, e.g., shaking waste packages or fault movement in the repository, will be investigated in separate calculations that might or might not include uncertainty and variability.

Volcanism will be investigated in a separate calculation. Intrusion plumbing, enhanced waste-package degradation, waste entrainment, or airborne dispersal might be handled probabilistically.

Inadvertent human intrusion will be evaluated for TSPA-VA by looking at one deterministic scenario—waste falling down a drill hole into the saturated zone.

For criticality, only the changes in the source term are likely to be investigated in a full TSPA calculation; other effects will be considered in side calculations. Size and duration of the criticality might be specified probabilistically. Different locations, e.g., within a waste package or in the UZ, might be considered.

7.4 SENSITIVITY ANALYSIS FOR TSPA-VA

In addition to evaluating the performance and associated uncertainty for the reference repository design and various alternative designs, another important goal of TSPA-VA is to determine what facets of the engineered and natural systems have the most influence on repository performance, and thereby to provide input to the design and site-characterization organizations regarding where additional data are needed and would provide the greatest increase in confidence about the repository. And beyond this formal goal, there is the simple need to understand the results and make them clear to all interested parties. A number of methods will be used to explain the results and quantify the sensitivities.

7.4.1 Methods for Sensitivity Analysis

The purpose of sensitivity analysis, also called uncertainty importance analysis, is to determine the parameters or components of the system which most influence the final results (i.e., the measures of performance). In a practical sense this is a function of both sensitivity (i.e., if a parameter is varied, how much do the performance measures change) and uncertainty (i.e., how much variation of a parameter is reasonable). For example, there could be a parameter to which the results are very sensitive, but which is exactly known. For practical purposes, that parameter would not be regarded as important. Of course, the determination of which parameters or components are most important depends on the particular performance measure being used. This was clearly demonstrated in TSPA-1993 (Andrews et al., 1994; Wilson et al., 1994) and TSPA-1995 (M&O, 1995), where it was shown that the important parameters are different for 10,000-year peak doses than for million-year peak doses, for example. Some methods for investigating sensitivity are discussed below.

Scatter plots. Scatter plots are a good qualitative method of looking for sensitivities. The final results (i.e., the performance measures obtained from a Monte Carlo simulation) are plotted against the input parameters and visually inspected for trends (it can be worthwhile to look at both linear and logarithmic axes). If there is a visible trend, it is an indication of sensitivity. The performance measures can also be plotted against various subsystem quantities or surrogate performance measures (e.g., groundwater travel time or waste-package lifetime) to determine whether that subsystem or performance surrogate is important to performance. These qualitative results can be made more quantitative by calculating correlation coefficients or by regression analysis.

Regression analysis. In regression analysis, a mathematical relationship between the outputs (performance measures) and inputs (model parameters) of a Monte Carlo simulation is developed. Typically, a method called stepwise linear regression is used, in which only a subset of the input parameters is used for the regression, with parameters added one at a time based on calculated correlation coefficients. Parameters that have little influence on the performance measure are those whose addition only marginally changes the variance of the output. Linear regression can be done with raw values, logarithms, or rank values (1 for the lowest value, 2 for second lowest, etc.) to see which one produces the best correlations. This method produces a ranking of input parameters according to their impact on the performance, and a quantitative measure of the impact (basically, the correlation coefficient for the performance measure vs. the input parameter).

In past TSPAs, a number of the model parameters have been highly correlated, e.g., fracture flux and overall infiltration flux or seepage flux and overall infiltration flux. As a result of these input correlations, the standard stepwise regression model does not give a unique solution. In particular, the usual importance criteria, such as the standard regression coefficients, order-of-entry of the variables, on the increment in R^2 when a variable enters the model, are invalid indices for the importance ranking. Instead, the partial correlation coefficients (PCCs) should be used to decide when to add a parameter to the model, and these provide the correct importance ranking when the model is completed (Ramarao et al., 1997).

Differential analysis. Another quantitative method for ranking important parameters is differential analysis, in which the partial derivatives of the performance measure with respect to the input parameters are calculated in order to find out how much performance is affected when one parameter is varied while the others are held constant. The partial derivatives can be normalized in such a way as to provide a measure of importance. A significant drawback of this method is that it is local—the derivatives are calculated about a point in the parameter space, and only represent the sensitivity at that point. In contrast, regression analysis of Monte Carlo results is more global—the sensitivities are determined and ranked taking into account the whole parameter space. Also, differential analysis requires additional calculations, while regression analysis uses the same calculations that are done for the uncertainty analysis (that is, the calculations from the Monte Carlo simulations).

Alternative models or parameter sets. A useful but less systematic method of sensitivity analysis is to look at discrete cases: perhaps some discrete sets of input parameters (as opposed to a systematic sampling) or perhaps some discrete choices of alternative models for a given process or subsystem. This method provides qualitative information about the sensitivity to the changes in assumptions (do the results change a little or a lot?), but not a quantitative ranking of the type produced by the previous two methods (see Section 7.3).

The above methods, with the exception of differential analysis, have been used extensively in previous TSPAs, and will be used extensively in TSPA-VA. Differential analysis is less useful because of the drawbacks mentioned above (see also Helton et al., 1991). It may be used in a limited sense (for example, to study how variations of a few particular parameters affect the results), but will not be used systematically for TSPA-VA. Studies examining alternative models and parameter sets are being done on two levels:

1. Many sensitivity studies looking at variations in assumptions are being done in the preliminary work that is being used to decide on the final form of the models and parameter sets for TSPA-VA. For the most part, these studies are being done at the subsystem or process level, not with the total-system model. Many such studies are defined in the analysis plans that came out of the various abstraction/testing workshops.

2. Some alternative models or parameter sets will be examined at the total-system level, including full Monte Carlo simulation. This will be done only for a limited number of the most important alternatives. The alternatives being considered for the various TSPA components are discussed in Chapter 6 and Section 7.3. In TSPA-VA, this type of analysis is what is meant when a "sensitivity study" or "sensitivity case" is mentioned.

7.4.2 Approaches to Making the Results More Understandable

It has been a strong recommendation of outside review groups that much more supporting analysis should be presented to make the TSPA results more understandable. Without additional information, a CCDF of results does not convey much understanding. In addition, it has been recommended that the TSPA results be presented in a more readable fashion to a broader audience. Some proposed methods to help make the results more understandable follow.

Time plots for particular realizations. The TSPA peer-review group has recommended that extensive amounts of time-evolution information should be presented to aid in understanding the results (Budnitz et al., 1997). They recommended plotting over time such information as waste inventory, temperature, humidity, in-drift chemistry, corrosion rates and degree of penetration of waste packages, waste-form degradation, rates of mobilization of radionuclides, UZ radionuclide-transport time, SZ dilution and radionuclide-transport time, release rates of radionuclides into the biosphere, and population and lifestyle assumptions. In past TSPAs (e.g., M&O, 1995) emphasis has been on showing time histories for a realization in which all sampled parameters take their mean values. It would additionally be useful to present one or more realizations with high releases and one or more realizations with low releases (perhaps pick out the tenth-percentile and ninetieth-percentile realizations, for example, or the $\mu\pm1\sigma$ and $\mu\pm2\sigma$ realizations—see Section 7.3.3). By examining the differences between these different realizations in detail, the conditions necessary to produce high releases could be better understood.

Subsystem measures. It can be very useful to examine subsystem performance to understand better what the various parts of the system are contributing to overall performance. For example, looking at residence time or transport time in different parts of the system (e.g., engineered-barrier system, unsaturated zone, saturated zone) can help to explain the overall results as well as providing an indication of which subsystems are most important to performance. Looking at cumulative releases, release rates, or concentrations at various locations (e.g., at the waste form, outside the waste package, at the edge of the EBS, at the water table, at the water-withdrawal point) can likewise help to show the relative importance of different barriers.

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Table 7.1-1. Key Information from Various TSPA-VA Models.

Model/Code	Abstraction
Climate Model (expert judgement)	Change in infiltration as f(x, t) for various future climate scenarios
UZ Flow Model (TOUGH2)	Multiple, 3-D and 2-D ambient flow fields [fracture/matrix velocity and flux as f(x,t)] for various uncertainties in flow parameters and infiltration
Mountain-Scale Thermohydrology (TOUGH2)	Scaling factors for drift-scale thermo-hydrology model as a function of parameter/model uncertainty
Drift-Scale Thermohydrology (NUFT)	Temperature, relative humidity, liquid saturation as f(x, t, design, conceptual model)
Drift-Scale Seepage (combination of various models: TOUGH2, NUFT, analytical models)	Seepage flux into drift as a function of far-field percolation, temperature, and uncertain parameters.
Near Field Geochemistry (EQ3/6, AREST-CT)	Change in chemical composition with (x, t) in EBS for various fluid/materials scenarios
Waste Package Degradation (WAPDEG)	First pit penetration and pit growth rate as f(x, t, T, RH, Cl^-, design)
DHLW Waste-Form Degradation (AREST-CT)	Glass degradation as f(t, T, RH, chemical composition)
CSNF Waste Form Degradation (AREST-CT)	CSNF degradation as f(t, T, RH, chemical composition)
Waste-form mobilization/EBS Transport (RIP, AREST-CT)	Radionuclide mass flux out of EBS and into UZ far-field for various and design and thermal-chemical-hydrologic scenarios
Rockfall model (design analyses)	Size, frequency of rockfall
Unsaturated-Zone Transport (FEHM)	Radionuclide mass flux rate from UZ to water table as f(x,t) as a function of parameter and model uncertainty
SZ Flow/Transport (FEHM)	Concentration and flux as f(x, t) at 20 km downgradient (unit-response breakthrough) as a function of model/parameter uncertainty
Biosphere (GENII)	BDCFs for selected radionuclides as a function of climate and model/parameter uncertainty
Criticality (MCNP)	Increase in inventory with time at (x, t)
Disruptive events (expert judgement)	Frequency and consequence of event

Table 7.3-1. Generalized Base Case Information

Domain	Base Case (design/process/models/B.C.)
Design	concrete liner
	2-layer waste package
	no backfill
	steel pedestal
	concrete invert
	85 MTU/acre; point loading
UZ Flow	LBNL base-case model (calibrated to site data): - 3-5 infiltration maps - 3-D DKM
Climate change	alternating time sequence of three steady states: dry climate; long-term average; and super-pluvial
Waste Inventory	10 radionuclides with the highest dose: -CSNF -DHLW -DOE SNF -Naval Fuel
Thermohydrology	use base-case design, hydrogeology, waste stream, and rockfall models; ECM model with reduced matrix satiation
	mass loading only for CSNF
	DHLW placed between CSNF
	some consideration for DOE SNF (TBD) and Naval fuel
Rockfall	drift closure as f(t) (TBD): probably a step function for closure of the drift
Near Field Geochemical Environment	use base case design
	fluid/mineral compositions as a function of time for 6 locations in NFE
	gas compositions as a function of time for 6 locations in NFE
	microbial effects
Waste Package Degradation	use WAPDEG (include pH, Cl, T, RH, microbial, and O2 effects)
	use WPDEE to extent possible
	humid air corrosion
	aqueous corrosion (drips and water film)

Table 7.3-1. Generalized Base Case Information (continued)

	no dry oxidation
	patches approach to package corrosion
	no galvanic protection
	spatial variability in environments (q_{perc}, T, RH, S_l) -dripping zones (%TBD) -non-dripping zones (%TBD) -multiple temperature zones (# TBD)
Waste Form Degradation	CSNF: Steward/Stout model
	DHLW: glass dissolution model
	Cladding degradation model
EBS Transport	Conca diffusion model
	Advection (drip) model: seepage models for flow around packages and through packages (based on several alternative seepage models for flow into the drifts)
UZ Transport	FEHM particle tracking coupled with RIP
	K_d approach to rock-water-colloid interactions
SZ Flow/Transport	Breakthrough response curves developed from 3-D FEHM flow/transport site-scale model and unit step function input; convolution of unit breakthrough curves with actual UZ releases at water table
Biosphere	BDCF's from M&O/SAIC implemented in RIP
Disruptive Events	None

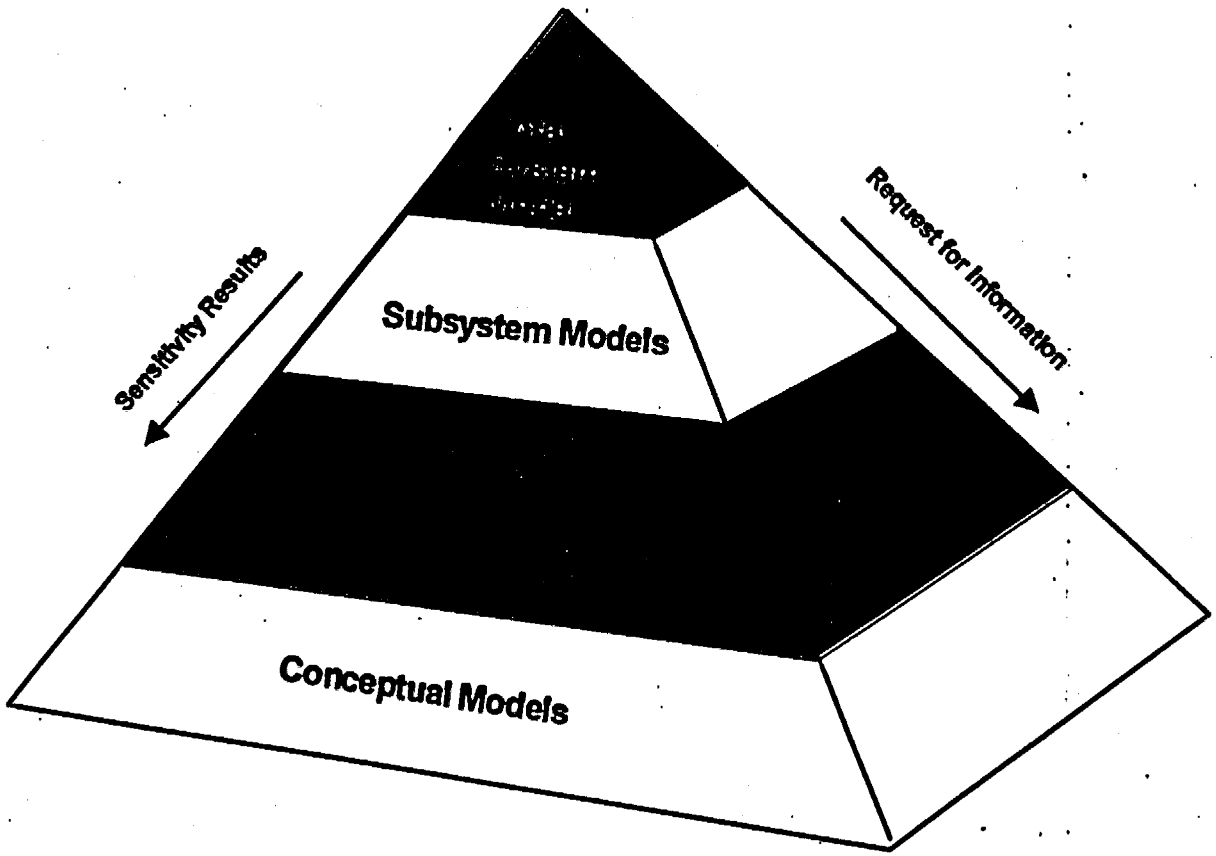

Figure 7.1-1. Total System Performance Assessment Model Hierarchy

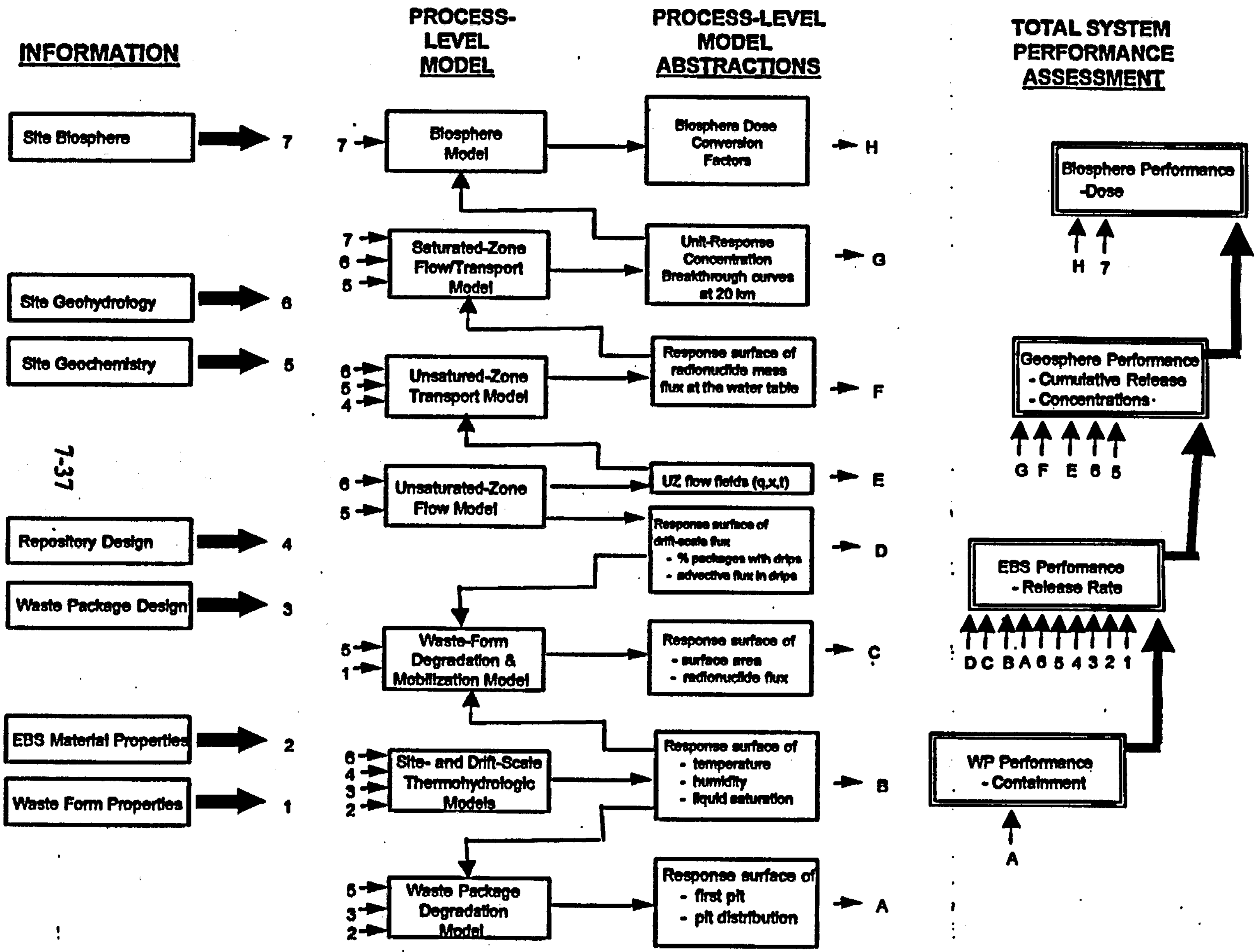

Figure 7.1-2. Overall Information Flow Diagram for TSPA-VA

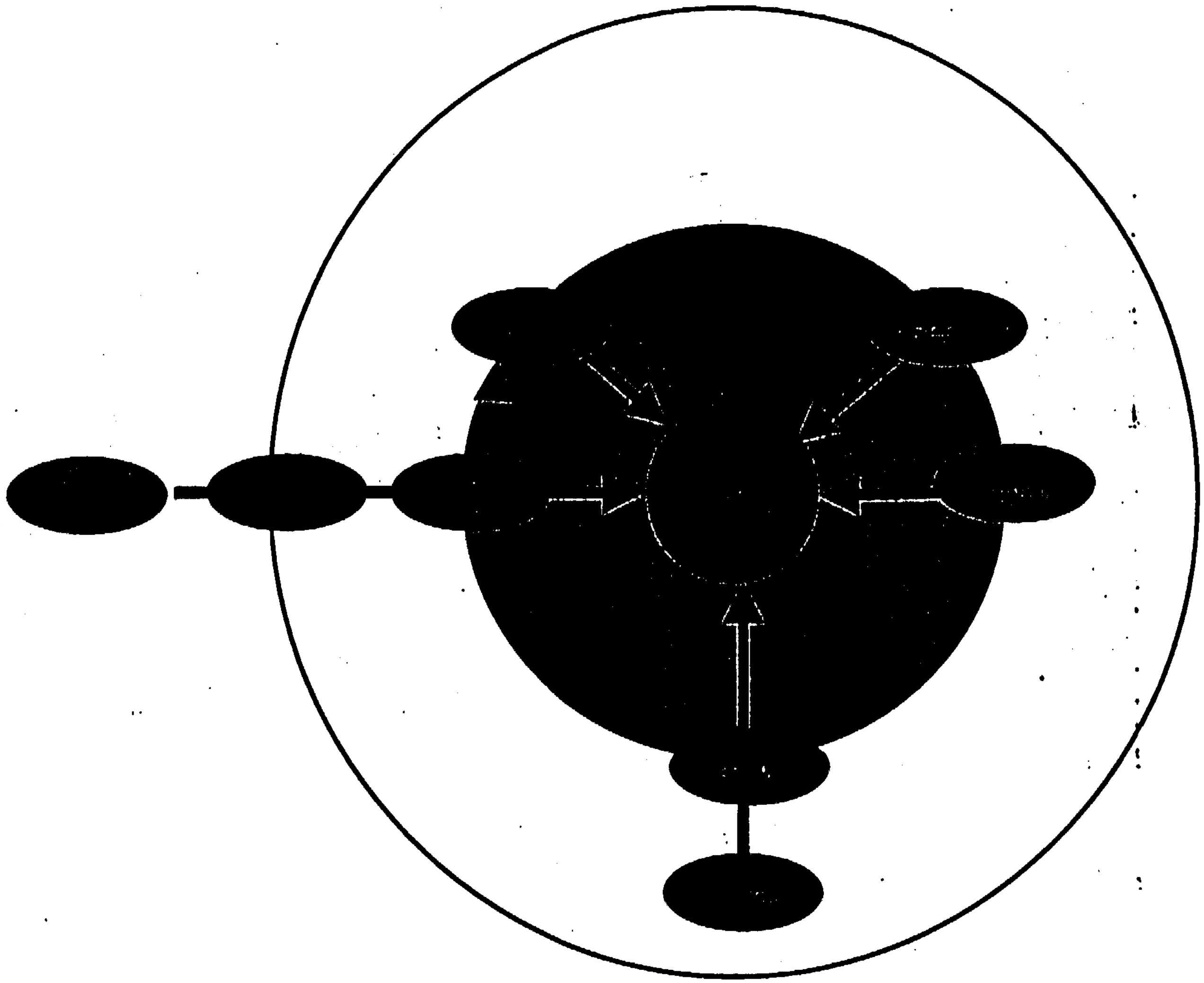

Figure 7.1-3. General Code Architecture for TSPA-VA

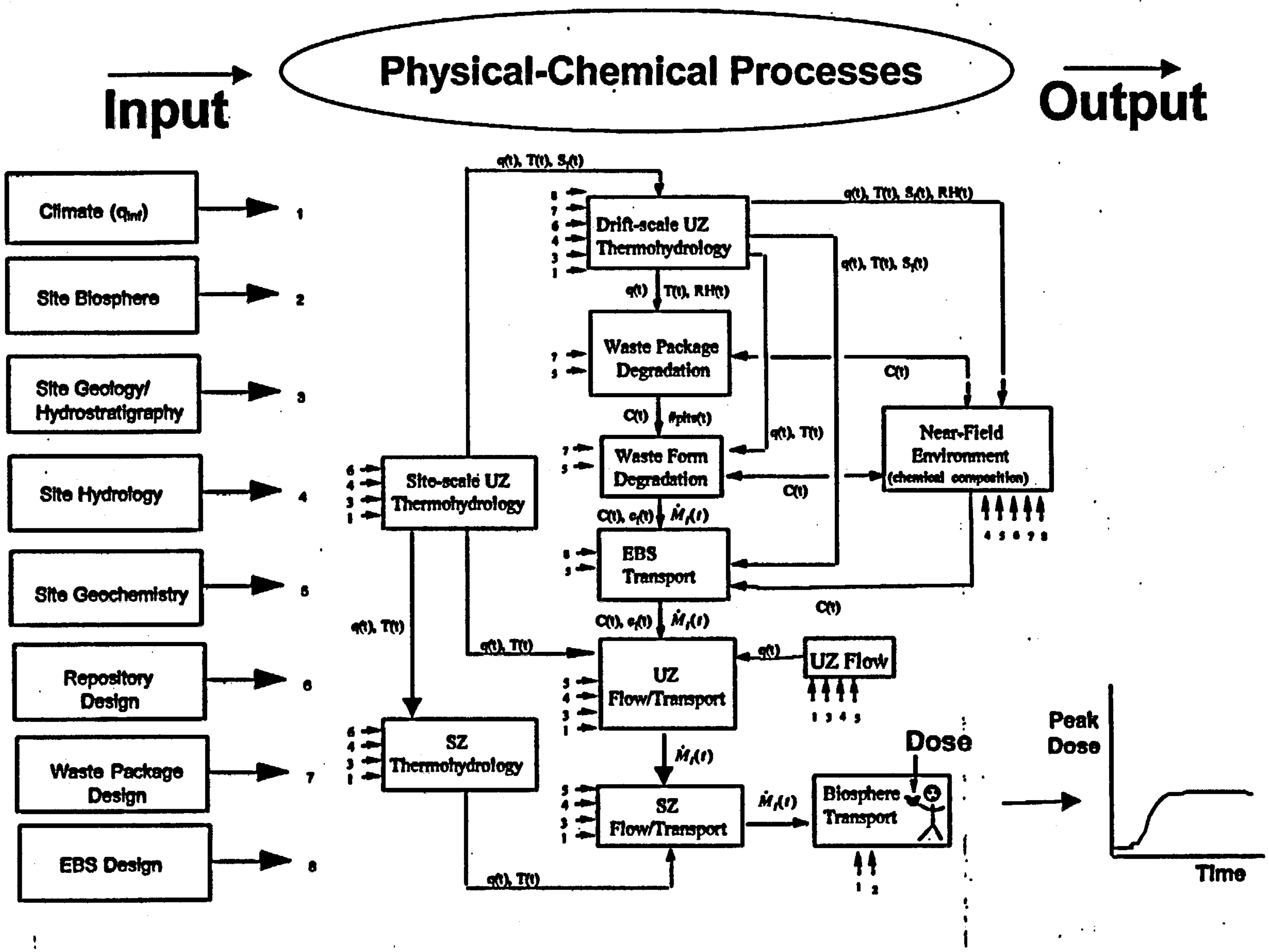

Figure 7.2-1. TSPA-VA Model Architecture

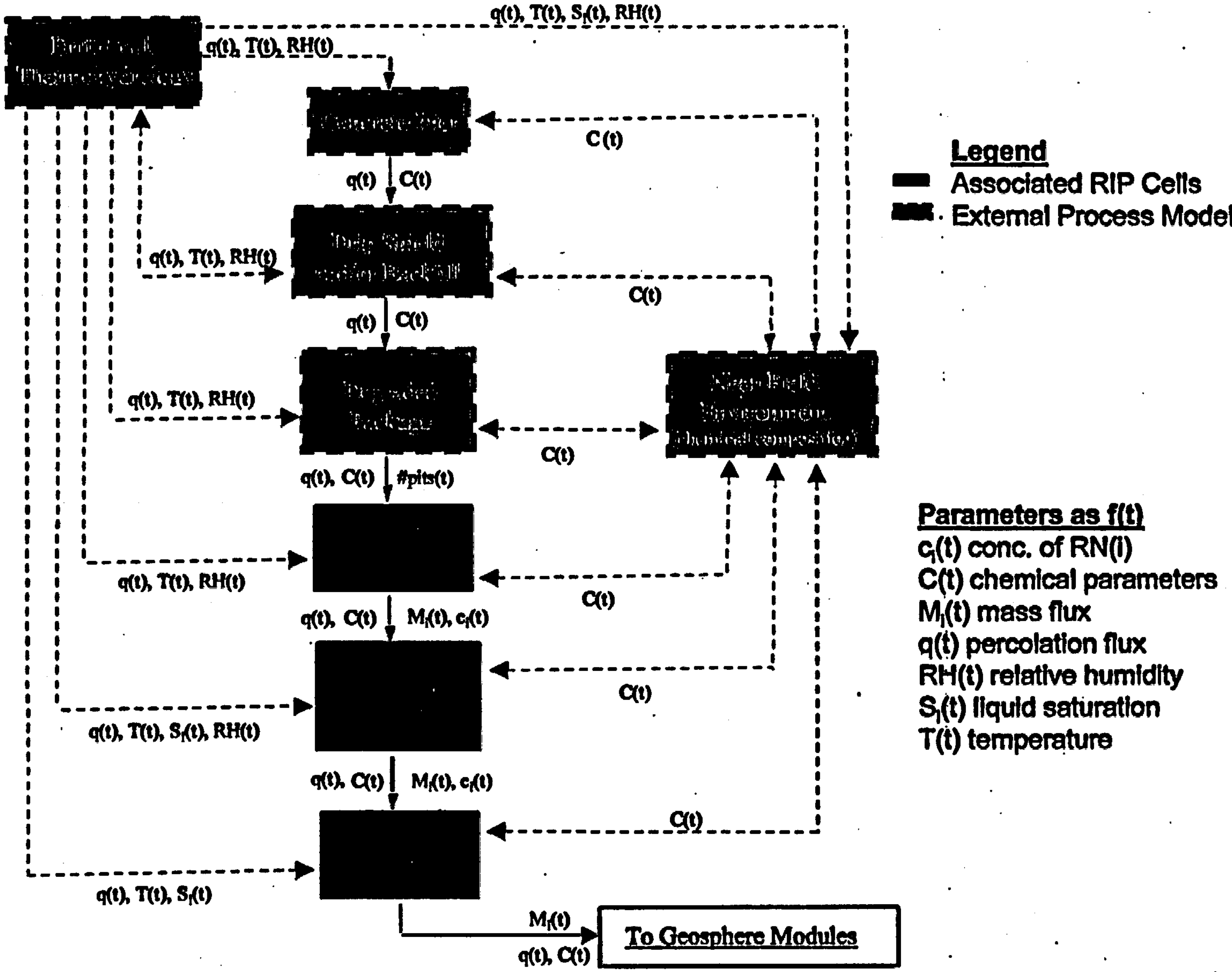

Figure 7.2-2. EBS model/code architecture for TSPA-VA, for a specific waste-package group.

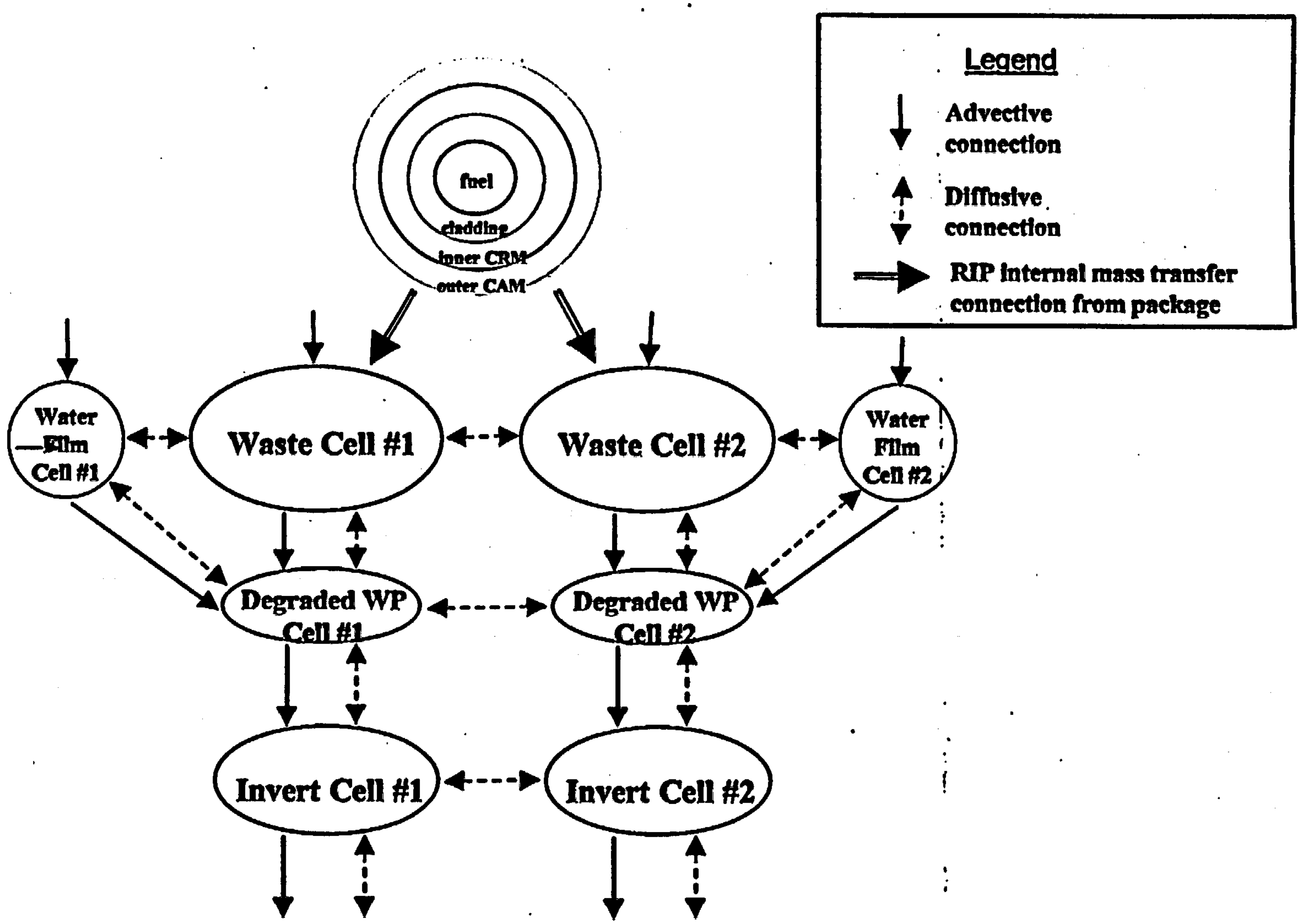

Figure 7.2-3. Schematic of associated cells in RIP used to represent processes in the EBS downstream and including the waste form.

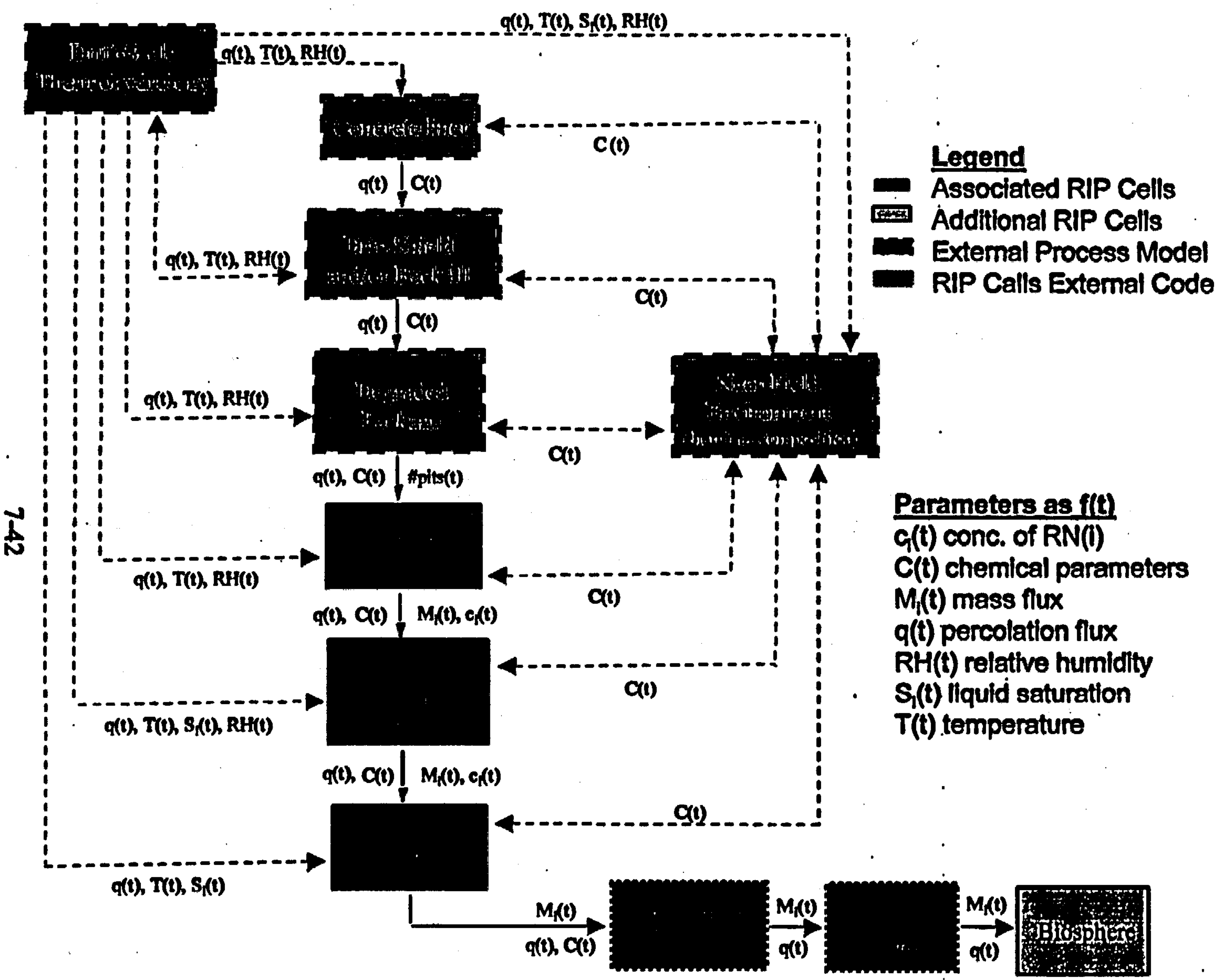

Figure 7.2-4. EBS and Geosphere Code Architecture for TSPA-VA

8.0 SUMMARY

Robert W. Andrews

This document started with a "big picture" look at TSPA-VA and its role in the context of the Viability Assessment of Yucca Mountain (Chapters 1 to 5), and then continued with detailed discussions of the abstraction of process models for input to the TSPA-VA (in Chapter 6) and the method of actually building the TSPA-VA model (in Chapter 7). It is now appropriate to step back and re-look at the TSPA-VA in its entirety. In particular, it is useful to re-examine the range of different "users" of TSPA-VA, discuss some of the major cross-cutting technical issues that weave through the analyses, and reiterate the general philosophy we are using in the generation and documentation of the TSPA-VA.

8.1 MAJOR USERS OF TSPA-VA

The primary use of TSPA-VA, which has been the emphasis of this document, is the legislatively-mandated use as being one of the four components of DOE's Viability Assessment. This objective is important because it will then be used by policy makers in their evaluation of the prospects for geologic disposal at Yucca Mountain. In addition to this objective, the results of the TSPA-VA, in particular the sensitivity analyses conducted to evaluate the significance of alternative models and designs, will be used as inputs to (1) the prioritization of additional scientific investigations, (2) the development of more detailed design descriptions and analysis, (3) a refocussing of DOE's Waste Containment and Isolation Strategy, (4) the draft and final Environmental Impact Statement, and (5) the planning for pre-licensing related discussions with the NRC. Each of these users is discussed below.

The TSPA-VA is an important component of the Viability Assessment. The Acting Director of the Office of Civilian Radioactive Waste Management, U.S. DOE, stated in his presentation to the NWTRB on June 25, 1997 in Las Vegas: "While the Viability Assessment is not one of the decision points defined in the Nuclear Waste Policy Act, its completion is expected to be significant to the development of a repository. The Viability Assessment will give policy makers key information regarding the prospects for geologic disposal at Yucca Mountain, and to justify its continued funding of the program if it is warranted." These policy makers will use TSPA-VA results and conclusions directly and will also solicit input from a range of different reviewers of the document. We need to be able to communicate the TSPA-VA at varying levels of detail to assure that the range of possible reviewers understand the implications of the analysis.

A key use of the TSPA-VA is to identify the additional scientific investigations that are needed to move from the Viability Assessment to a successful License Application. Again, as the Acting Director stated to the NWTRB: "The Viability Assessment also serves as an important management tool for the program. The development of the components will help integrate the ongoing activities and assembled information will guide the completion of the site characterization by identifying those areas where additional scientific and technical work is required to evaluate the site, to prepare a defensible, complete, cost-effective and timely license application." Previous TSPA analyses have also been used in this context.

A major use of performance assessment is to evaluate the performance implications of a range of design alternatives. These design sensitivity analyses may be used either with respect to the additional safety afforded by the design feature given the "expected" or "nominal" repository system behavior or the added confidence the design feature provides in compensating for uncertain site conditions. In order for management to make informed decisions on alternative designs, they must be aware of the uncertainties in the behavior of the design features, the expected performance implications of the design features, and the possible costs associated with implementing these features. Some of the key design alternatives we intend to evaluate in TSPA-VA include the use of backfill, ceramic or other impervious drip shields placed on the waste package, and ceramic coatings on the waste package.

Another use of the TSPA-VA is to update the Waste Containment and Isolation Strategy. This strategy essentially defines the key elements of the "safety case" that would be put forward in the licensing process. The degree of confidence in the various components of the system, combined with the significance of each component to the overall system behavior, will be a major aspect of the revised strategy, just as the results of earlier TSPA analyses were instrumental in the generation of the current strategy (DOE, 1996).

Additional TSPA sensitivity analyses are required to address specific issues that need to be examined in the Environmental Impact Statement (EIS). The scope of the Yucca Mountain repository EIS includes a comprehensive evaluation of the environmental impacts associated with constructing, operating, and closing a proposed high-level radioactive waste repository at Yucca Mountain. Of particular interest in the EIS are the potential environmental impacts of alternative inventories [notably all commercial spent nuclear fuel, all DOE spent nuclear fuel and high-level waste, DOE special-performance-assessment-required waste, commercial greater-than-class C waste, and additional plutonium surplus fissile materials, in addition to the base case inventory of 70,000 metric tons of heavy metal (MTHM)] and different areal mass loadings of the repository [in particular a low and intermediate thermal load, defined as 36 and 60 MTHM per acre, respectively, in addition to the base case of 85 MTHM per acre]. These sensitivity analyses will be complementary to the TSPA-VA and documented in the EIS.

Finally, the TSPA-VA analysis will continue to be an important vehicle for continued pre-licensing dialog with the Nuclear Regulatory Commission. The NRC has refocussed their prelicensing repository program on the resolving the issues most significant to repository performance. These issues are called key technical issues (KTIs). It is important for DOE's TSPA-VA to address these same issues and evaluate their potential significance to performance so that there is a common understanding of the basis for additional technical work needed to resolve these issues.

8.2 MAJOR CROSS-CUTTING TECHNICAL ISSUES

As each of the abstraction activities was described in Chapter 6, individual issues associated with each process model were outlined and an approach identified for addressing that issue within the context of TSPA-VA. While it is necessary to go into this detail, it is also useful to examine the common issues that run through many of the process models. There are two major issues that most significantly affect the predicted performance of the Yucca Mountain repository system: the predicted distribution of moisture in the rock and the predicted degradation of engineered materials. Each of these is discussed below.

The movement of moisture (both liquid and vapor phase) around, into, and within the emplacement drifts, through the unsaturated zone, and into the saturated zone has been identified as a key driver in every TSPA conducted of the Yucca Mountain site. Of particular interest is the distribution of percolation flux in the host rock at the repository depth. This distribution includes spatial and temporal components as well as the division of this flux between fractures of varying carrying capacity and the rock matrix. The fraction of the percolation flux that seeps into the drifts and the fraction of that seepage that actually encounters a waste package will be key determinants in the timing and rate of release of radionuclides from the engineered barriers to the natural system. These values are also dependent on the fracture and matrix characteristics and the degree of coupling of the flow between these two media. The flux and rock characteristics also significantly impact the thermal and hydrologic response of the system to the heat generated by the wastes, which in turn affect the degradation of the engineered components. Flow and radionuclide transport in the unsaturated and saturated zones beneath the repository also depend on the flow characteristics of the geologic media. All of the above process models must address the impact of the uncertainty in the flux and rock characteristics on the overall performance.

The prediction of how the engineered materials to be emplaced in the repository will behave over very long time periods is as important to the overall performance as is the description of the moisture distribution. The desire is to contain the radionuclides in the engineered system for as long as possible and then to allow only a slow release from the engineered system. Several redundant materials are in the current reference design (M&O, 1997), including a corrosion allowance material for the outer barrier of the waste package, a corrosion resistant material for the inner barrier of the waste package, the Zircaloy cladding, and the ceramic waste form itself. Other materials, including ceramic drip shields or coatings on the waste package, are also being considered as design options. All of these materials will degrade by aqueous corrosion and other processes. Predictions of the lifetimes of such materials over the time frames of interest (tens of thousands of years) will be based to a large extent on the extrapolation of short-term laboratory experiments. The applicability and uncertainty associated with these extrapolations significantly affects the confidence in the predicted behavior of the engineered components.

8.3 GENERAL PHILOSOPHY

The basic philosophy and general methodology and approach to be used in TSPA-VA is essentially unchanged from what was employed in previous TSPA iterations. The primary difference in this iteration is the heightened expectations (discussed above) and the objective to be much more of an integrating analysis of our current understanding, rather than simply an assessment of the impact of a range of uncertain components. While uncertainty still remains, some of which we are attempting to quantify through the use of formal expert elicitations, we have strived to base our models on the wealth of observations and data available for each of the key processes that need to be quantified in the assessment of the future behavior of the system.

Many of the comments received about previous TSPA analyses have focussed on the technical basis for the assumptions made in the analysis and the presentation of the results. Our desire is to make the TSPA analysis and documentation both "traceable" and "transparent", while also recognizing that there are different audiences from very different backgrounds that will review the documentation. Although meeting the expectations of all reviewers in a single document will be difficult, we are striving to generate the report in a fashion that will allow all interested individuals to have a degree of confidence in the analysis, the supporting technical/scientific basis, the ramifications of the uncertainty to future scientific and engineering studies, and the determination of the viability of the Yucca Mountain repository system.

The focus of the TSPA-VA analyses will be on determining the "probable behavior" of the repository system, as we defined in Chapter 7. While there may be a tendency to equate this to the term "reasonable assurance" as used in the language of NRC regulations, this is not the intent at this stage. While the "probable" or "expected" behavior is an important input to the determination of "reasonable assurance", the Nuclear Regulatory Commission recognizes that any assessment of "probable behavior" has associated with it uncertainty. Therefore, it is expected that eventually we may want to explore reasonably "worst-case" or "bounded" performance predictions, as well as a range of defense-in-depth engineered-barrier designs that could be used to compensate for the possibility of such "unexpected" conditions. The NRC anticipated this in their Statements of Consideration (NRC, 1983) that accompanied the regulatory requirements in 10 CFR Part 60:

> The Commission anticipates that licensing decisions will be complicated by the uncertainties that are associated with predicting the behavior of a geologic repository over the thousands of years during which HLW may present hazards to public health and safety. It has chosen to address this difficulty by requiring that the DOE proposal be based upon a multiple barrier approach. An engineered barrier system is required to compensate for uncertainties in predicting the performance of the geologic setting, especially during the period of high radioactivity. Similarly, because the performance of the engineered barrier system is also subject to considerable uncertainty, the geologic setting must be able to contribute significantly to isolation.

TSPA-VA will look at the "probable behavior" of the overall repository system. However, it will be possible to evaluate the relative contribution of the engineered and natural system of barriers to the overall system performance through the various "time slices" we will present, showing the predicted future behavior of the various system components. We recognize that the TSPA-VA is an important stepping stone to the TSPA-LA. The TSPA-LA will benefit from the review comments we receive from all interested parties on the TSPA-VA document, from feedback received during presentation to the public and interested organizations, as well as from additional site and engineering data and analysis and continued pre-licensing dialog with the NRC.

8.4 REFERENCES

U.S. Department of Energy (DOE), 1996. Highlights of the U.S. Department of Energy's Updated Waste Containment and Isolation Strategy for the Yucca Mountain Site, YMP/96-01, U.S. Department of Energy, Office of Civilian Radioactive Waste Management, Washington, D.C.

Civilian Radioactive Waste Management System Management and Operating Contractor (M&O), 1997. Reference Design Description for a Geologic Repository, B00000000-1717-5707-00002, Rev. 00, Las Vegas, NV.

U.S. Nuclear Regulatory Commission (NRC), 1983. Statements of Consideration for 10 CFR Part 60, 48 FR 28194, U.S. Nuclear Regulatory Commission, Washington, D.C.

Nuclear Waste Technical Review Board (NWTRB), 1997. Report to the U.S. Congress and The Secretary of Energy - 1996 Findings and Recommendations, Arlington, VA.

Codes and Regulations:

10 CFR Part 60 (Code of Federal Regulations), 1990, Title 10, Energy, Part 60, Disposal of High-Level Radioactive Waste in Geologic Repositories, U.S. Government Printing Office, Washington, D.C.

DRAFT DISCLAIMER

TRW

RW Environmental
Safety Systems Inc.

1180 Town Center Drive
Las Vegas, NV 89134
702.295.5400

WBS: 1.2.3.12.5
QA: N

Contract #: DE-AC01-91RW00134
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August 19, 1997

Stephan J. Brocoum, Assistant Manager
for Licensing
U.S. Department of Energy (DOE)
Yucca Mountain Site Characterization Office
P.O. Box 30307
North Las Vegas, NV 89036-0307

Attention: Technical Publications Management

Dear Dr. Brocoum:

Subject: Completion of Level 3 Fiscal Year (FY) 1997 M&O Milestone SP3000M3, "Near Field and Altered-Zone Environment Report Volume I: Technical Bases for EBS Design, Revision 1," Work Breakdown Structure (WBS) 1.2.3.12.5

Three copies of the above-referenced deliverable are being submitted for deliverable acceptance review in accordance with YAP-5.1Q. This action completes delivery of Milestone SP3000M3. A second YAR form is also included for the related deliverable SPL5DM4. This YAR may be approved when acceptance of SP3000M3 is completed.

If you have any questions regarding this deliverable, please contact Dwight Hoxie at (702) 295-5740, or me at (702) 295-5604.

Sincerely,

Larry R. Hayes

Larry R. Hayes, Manager
Site Evaluation Program Operations
Management and Operating Contractor

LRH/clt

Enclosures:
(1) Deliverable Acceptance Review Forms
(2) Participant Planning Sheet
(3) Milestone SP3000M3

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M. D. Voegele, M&O, Las Vegas, Nevada MD Voegele
LV RPC = 193 pages (previously processed)

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D. T. Hoxie, M&O, Las Vegas, Nevada
G. J. Lindenburg, DOE/YMSCO, Las Vegas, Nevada

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