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Civilian Radioactive Waste Management System
Management & Operating Contractor

Total System Performance Assessment–Site Recommendation Methods and Assumptions

TDR-MGR-MD-000001 REV 00 ICN 01

October 1999

Prepared for:

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September 1999

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CHANGE HISTORY

Revision Number	Interim Change No.	Effective Date	Description of Change
0	0	09/03/99	Initial issue.
0	1	10/30/99	Provides update in response to the U.S. Department of Energy and YAP-30.12, *Publications Review, Approval, and Distribution* review. The results, conclusions, and recommendations did not change; however, the contents were changed and supplemented to clarify and expand on the discussions provided in REV 00. Pages affected are: 1-3, 1-7, 1-16, F1-1, 2-2, 2-3, 3-13, 3-21, 3-35, 3-86 and 5-4. Pages added are: iva, ivb, 5-4a, and 5-4b.

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ACRONYMS AND ABBREVIATIONS

3-D	three-dimensional
AMR	Analysis and Model Report
BDCF	biosphere dose conversion factor
BWR	boiling water reactor
CAM	corrosion allowance material
CCDF	complementary cumulative distribution function
CDF	cumulative distribution function
CHLW	commercial high-level radioactive waste
CRM	corrosion resistant material
CRWMS M&O	Civilian Radioactive Waste Management System Management and Operating Contractor
CSNF	commercial spent nuclear fuel
DFEP	disruptive features, events, and processes
DOE	U.S. Department of Energy
DST	drift scale heater test
DSNF	DOE-owned spent nuclear fuel
EBS	engineered barrier system
EFEP	expected features, events, and processes
EIS	Environmental Impact Statement
EPA	U.S. Environmental Protection Agency
ESF	Exploratory Studies Facility
FEP	feature, event, or process
HIC	hydrogen induced cracking
HLW	high-level radioactive waste
ICRP	International Commission on Radiological Protection
IDGE	in-drift geochemical environment
INEEL	Idaho National Environmental and Engineering Laboratory
IRSR	Issue Resolution Status Report
KESA	key elements of subsystem abstraction
LA	license application
LHS	Latin hypercube sampling
LLNL	Lawrence Livermore National Laboratory
MTHM	metric tons of heavy metal
MTU	metric tons of uranium

NAGRA	National Cooperative for the Disposal of Radioactive Waste (Switzerland)
NAS	National Academy of Sciences
NEA	Nuclear Energy Agency
NEPO	Natural Environment Program Operations
NRC	U.S. Nuclear Regulatory Commission
NTS	Nevada Test Site
NWTRB	U.S. Nuclear Waste Technical Review Board
PAO	Performance Assessment Operations
PAPR	Performance Assessment Peer Review
PMR	Process Model Report
PWR	pressurized water reactor
QA	quality assurance
SCC	stress corrosion cracking
SHT	single heater test
SNF	spent nuclear fuel
SR	site recommendation
SZ	saturated zone
TEDE	total effective dose equivalent
TH	thermal hydrologic
THC	thermal-hydrologic-chemical
THM	thermal-hydrologic-mechanical
TM	thermal mechanical
TSPA	total system performance assessment
TSPA&I	Total System Performance Assessment and Integration
TSPA-LA	Total System Performance Assessment–License Application
TSPA-SR	Total System Performance Assessment–Site Recommendation
TSPA-VA	Total System Performance Assessment–Viability Assessment
UZ	unsaturated zone
VA	Viability Assessment of a Repository at Yucca Mountain
WIPP	Waste Isolation Pilot Plant
YMP	Yucca Mountain Site Characterization Project

1. INTRODUCTION

1.1 BACKGROUND

As mandated in the Nuclear Waste Policy Act of 1982, the U.S. Department of Energy (DOE) has been investigating a candidate site at Yucca Mountain, Nevada, to determine whether it is suitable for development of the nation's first repository for permanent geologic disposal of spent nuclear fuel (SNF) and high-level radioactive waste (HLW). The Nuclear Waste Policy Amendments Act of 1987 directed that only Yucca Mountain be characterized to evaluate the site's suitability. Three main components of the DOE site characterization program are testing, design, and performance assessment. These program components consist of:

- Investigation of natural features and processes by analyzing data collected from field tests conducted above and below ground and from laboratory tests of rock, gas, and water samples

- Design of a repository and waste packages tailored to the site features, supported by laboratory testing of candidate materials for waste packages and design related testing in the underground tunnels where waste would be emplaced

- Quantitative estimates of the performance of the total repository system, over a range of possible conditions and for different repository configurations, by means of computer modeling techniques that are based on site and materials testing data and accepted principles of physics and chemistry.

To date, DOE has completed and documented four major iterations of total system performance assessment (TSPA) for the Yucca Mountain site: TSPA-91 (Barnard et al. 1992), TSPA-93 (Wilson et al. 1994; CRWMS M&O 1994), TSPA-95 (CRWMS M&O 1995), and the *Total System Performance Assessment–Viability Assessment* (TSPA-VA) (DOE 1998a, Volume 3). Each successive TSPA iteration has advanced the technical understanding of the performance attributes of the natural features and processes and enhanced engineering designs. The next major iteration of TSPA is to be conducted in support of the next major programmatic milestone for the DOE, namely the Site Recommendation (SR). The Total System Performance Assessment–Site Recommendation (TSPA-SR) will present a compliance evaluation of overall system performance against the guidelines and requirements in the revision of the DOE siting guidelines to be promulgated at 10 CFR 963, U.S. Nuclear Regulatory Commission (NRC) regulation for HLW disposal at proposed 10 CFR 63 (the proposed rule has been published at 64 FR 8640), and U.S. Environmental Protection Agency (EPA) environmental radiation protection standard to be promulgated at 40 CFR 197. At present, the NRC has issued the proposed 10 CFR 63 (64 FR 8640) for public comment whereas the EPA standard and the revised DOE siting guidelines are currently being developed. EPA has announced the release of 40 CFR 197 proposed rule on its website (www.epa.gov/radiation/yucca/rule.qui.htm) and the Federal Register announcement (which initiates the 90 day public comment period) is expected by the end of August, 1999.

The purpose of this document is to present the overall goals, objectives, scope, methods, approach, and assumptions to be used in the development of the TSPA-SR. This document will serve as a communication tool for coordinating the DOE TSPA activities and for keeping the NRC staff informed of the TSPA activities for the SR.

1.2 PLACING TOTAL SYSTEM PERFORMANCE ASSESSMENT–SITE RECOMMENDATION AND TOTAL SYSTEM PERFORMANCE ASSESSMENT–LICENSE APPLICATION INTO THE CONTEXT OF MAJOR U.S. DEPARTMENT OF ENERGY MILESTONES

Based on the technical findings of the *Viability Assessment of a Repository at Yucca Mountain* (VA), the DOE has concluded that Yucca Mountain continues to be a promising site for a potential geologic repository and that engineering studies should proceed to provide a comprehensive basis for agency decision making in 2001 on whether the site merits a recommendation to the President for development of a repository (DOE 1998b, Overview, p. 36). As identified in the VA, the following are the key Yucca Mountain Site Characterization Project (YMP) objectives (DOE 1998c, volume 4, p. 7-1):

- Publish a draft Environmental Impact Statement (EIS) in FY 1999. Completed in August, 1999.
- Complete the final EIS in FY 2000[1]
- If the site is suitable for development as a repository, complete the Secretary of Energy's SR to the President, accompanied by the final EIS, in FY 2001.
- If the President recommends the site to Congress, and Congress concurs, submit a license application (LA) to the NRC in FY 2002.

Complete TSPA analyses of the repository system are required for each of these major programmatic milestones, just as they were an integral part of the VA. The draft EIS TSPA analyses, which will be published in the very near future, have been based on the VA designs and models available at the time of the VA. The final EIS TSPA analyses will be based on the SR design and models that are being modified with new information collected since the completion of the VA.

The SR process begins with public hearings near Yucca Mountain to inform area residents that the Secretary of Energy is considering recommending the site. These public hearings are referred to as consideration hearings and will be announced in a federal register notice. These hearings are scheduled to be held in November 2000. The analyses and documents used to provide input for use in the consideration hearings constitute the report designated the Consideration Hearings Draft SR.

Following the consideration hearings, the Secretary of Energy will notify the governor and legislature of the State of Nevada and the affected Native American tribes regarding his decision on the SR. The information provided to these entities will consist of appropriate revisions to the

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[1] Current schedules, allowing for a 180-day comment period on the draft EIS, indicate the Final EIS would be completed in early FY 2001.

technical base available at the time of the consideration hearings based on comments received from the public, oversight groups, and other interested parties, as well as any new information (e.g., test results, analyses, models) that may have become available since the completion of the Consideration Hearings Draft SR.

The TSPA analyses and documentation that support the aforementioned major programmatic milestones are referred to as the TSPA-SR Revision 00 and TSPA-SR Revision 01, respectively. The reason for the nomenclature is to distinguish between the two analyses because they represent a phased approach to developing the technical basis for the Secretary of Energy's decision regarding whether or not to recommend the Yucca Mountain site to the President. In addition, the two TSPA iterations are only a few months apart, so only minor revisions in the analyses are anticipated, barring any unforeseen significant changes in analyses or models used as the technical basis for the TSPA analyses. Finally, the Revision 00 and Revision 01 identifiers are intended to indicate that the analyses shall be conducted and documented in accordance with a rigorous quality assurance (QA) process. Revision 01 of the TSPA-SR will respond to new information and to comments on Revision 00.

If the Yucca Mountain site is recommended by the Secretary of Energy and accepted by the President, the DOE will proceed to prepare a comprehensive LA for submittal to the NRC. An important component of this LA will be the postclosure performance assessment as required in the proposed 10 CFR 63 regulations (64 FR 8640). The TSPA analyses and documentation that would be prepared for this major program milestone shall be referred to as Total System Performance Assessment-License Application (TSPA-LA). Although the TSPA-LA may also undergo several revisions following the submission of the initial application, the focus would be on the initial submittal, currently planned for FY 2002 (assuming all the preceding milestones have been completed). The TSPA-LA will build upon the TSPA-SR Revision 01, incorporating the new field data and design information available at the time of the LA, comments received on earlier versions of the TSPA-SR analyses, and additional analyses specifically aimed at addressing particular NRC Key Technical Issues or acceptance criteria required in the NRC Yucca Mountain Review Plan.

1.3 OVERALL OBJECTIVES OF TOTAL SYSTEM PERFORMANCE ASSESSMENT–SITE RECOMMENDATION

1.3.1 Regulatory Guidance to Total System Performance Assessment–Site Recommendation

The objective of the TSPA-SR analyses is to provide a quantitative evaluation of the overall repository system's ability to achieve the postclosure performance criteria as specified in the repository siting guidelines identified by the DOE. The DOE's revised siting guidelines are expected to invoke the applicable implementing regulations set forth by the NRC. Until such time as the revised guidelines are available, the TSPA-SR will be guided by the available regulatory criteria in the NRC's proposed 10 CFR 63 (64 FR 8640).

The NRC, in their proposed 10 CFR 63 (64 FR 8640) has stated that "the results of performance assessment shall be the sole quantitative measure used to demonstrate compliance with the postclosure individual dose limit" (proposed 10 CFR 63, p. 8650 (64 FR 8640)). In particular, the proposed 10 CFR 63.102(j) (64 FR 8640) notes that "[d]emonstrating compliance with the postclosure performance objective specified at 63.113(b) requires a performance assessment to quantitatively estimate the expected annual dose, over the compliance period, to the average member of the critical group." In this context, performance assessment is defined in proposed 10 CFR 63.2 (64 FR 8640).

> "Performance assessment means a probabilistic analysis that:
>
> (1) Identifies the features, events and processes that might affect the performance of the geologic repository; and
>
> (2) Examines the effects of such features, events, and processes on the performance of the geologic repository; and
>
> (3) Estimates the expected annual dose to the average member of the critical group as a result of releases from the geologic repository" (proposed 10 CFR 63, p. 8665; 64 FR 8640).

In general, features, events and processes (FEPs) are natural or anthropogenic phenomenon, objects, structures, or conditions that have a potential to affect disposal system performance. (See Appendix A for full definition of FEPs.)

In conducting the analyses of postclosure performance, the NRC notes the need to take into account, as appropriate, the uncertainties associated with data, methods, and assumptions used to quantify the repository performance. The NRC has also acknowledged that, because of the uncertainties inherent in the understanding of the evolution of the geologic setting, biosphere, and engineered barrier system (EBS), proof that the geologic repository will be in conformance with the postclosure performance objective is not to be had in the ordinary sense of the word. They note that "what is required is reasonable assurance, making allowance for the time period, hazards, and uncertainties involved, that the outcome will be in conformance with the objective for postclosure performance of the geologic repository" (proposed 10 CFR 63.101(a)(2) (64 FR 8640)).

Evaluating compliance against the applicable federal regulations involves the use of complex predictive models that are supported by laboratory and field tests. These predictive models must be scientifically defensible and transparent. As noted by the NRC in the supplementary information accompanying proposed 10 CFR 63 (64 FR 8640), the defensible performance assessment (not the individual models), should contain:

1. A technical rationale for those features, events, and processes that have been included in the performance calculation as well as those that were considered but excluded
2. The specific attributes of the geologic setting, the engineered barriers, and the interactions between the natural and engineered barriers that represent a wide range of beneficial and detrimental effects on performance

3. A consideration of FEPs in light of available data and scientific understanding

4. An evaluation of alternative models consistent with the available data and scientific understanding

5. Reasonable and practical measures to ensure that the performance assessment provides a credible representation of a geologic repository at Yucca Mountain (proposed 10 CFR 63, p. 8650-8651 (64 FR 8640)).

In any evaluation of the performance of a complex system (such as the analyses required to address the ability of the Yucca Mountain repository system to meet the goal of protecting public health and safety and show compliance with applicable regulatory requirements), the analyst has many options to accommodate the inherent uncertainty associated with the complexity of the system. The analyst can use realistic and representative models of the FEPs incorporating uncertainty through probabilistic treatments consistent with the current state of scientific knowledge. Alternatively, where the models are complex, or the uncertainties are intractable, and defensible probabilistic characterizations are not available, the analyst may choose to develop a simplified bounding argument that is generally recognized as conservative. For each component model or parameter incorporated in the TSPA analyses of the Yucca Mountain repository system, these decisions must be clearly documented and defended.

1.3.2 Guidance from the Total System Performance Assessment–Viability Assessment Peer Review Panel for the Total System Performance Assessment–Site Recommendation

The panel, convened to conduct a Peer Review of the TSPA-VA, acknowledged that several different approaches can be taken to analyze complex processes in support of meeting the reasonable assurance requirements of the NRC. These approaches include:

- Improving and updating the component models
- Expanding the quality and quantity of data available to constrain model inputs
- Using bounding analyses (i.e., intentionally conservative assumptions, parameters and models)
- Design changes (Whipple et al. 1999, p. 40).

The Panel also notes that these four approaches are closely related and that the specific application of the approach depends on the nature of the process. For example, in cases where analytical approaches are available, significant improvements can be made by updating the component models and acquiring additional data to support the conceptualizations incorporated in the models. In the case of processes that may be essentially intractable, the only available option may be to treat these components through the use of bounding analyses or design changes (Whipple et al. 1999, p. 40). The TSPA conducted for the SR will take appropriate advantage of each of these four approaches.

The choice of when to use a bounding analysis (attempt to cover the deleterious effects on repository performance), and when to use a more realistic representation of a particular physical chemical process in the performance assessment is a function of the goal of the analysis and the degree of maturity of the process models. Again, as noted by the TSPA-VA Peer Review Panel (Whipple et al. 1999, p. 41), because the use of bounding analyses produces results that are in a conservative (lower performance) direction, they are generally assumed to be highly credible by regulatory agencies. In addition, such analyses are commonly less data intensive than those conducted on a more realistic basis and therefore are useful when the existing analytical capabilities have deficiencies that would be difficult and time-consuming to correct. Therefore, the Panel concluded that bounding analyses would appear to be especially appropriate as the Project approaches the preparation of the TSPA-LA[2]. The Panel continues by noting that the bounding analyses must also be defensible and that care should be taken to ensure that unacceptably conservative projections of repository performance do not result. This last observation is interpreted to imply that unnecessarily conservative assumptions should not unduly bias the overall safety strategy.

1.3.3 Total System Performance Assessment–Site Recommendation Analyses

The analysis plans for the TSPA-SR are being designed with sufficient flexibility that a range of parameters and models can be used to describe each component of the system in the assessment. To the extent feasible, the realistic representation of parameters and models are being developed to describe the most realistic, best-estimate, or probable behavior of the system, and incorporate a realistic and reasonable description of the uncertainty in that representation to determine the expected performance of the system. In some components, a conservative bounded approach that uses intentionally conservative assumptions, parameters, and models may be required for those components of the system that are highly complex, or lack sufficient data for defensible definition. Defensibility, in this sense, refers to models and data that can be defended in a regulatory environment on the basis of information available for use in the SR at the time it is submitted. Using such conservatisms has the benefit of removing overly complex, and sometimes intractable, uncertainties from having to be considered explicitly.

Given that TSPA-SR will include components with both realistic and conservative bounding, it is worthwhile to quote from the TSPA-VA Peer Review Panel Final Report (Whipple et al. 1999, p. 44):

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

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[2] The Final Report of the TSPA Peer Review Panel had as an objective to provide suggestions for moving toward the TSPA-LA (Whipple et al. 1999, p. 14). Although the goals of the LA are different than the SR, it may be assumed that the amount of scientific evidence required for the decision makers to make reasonably informed decisions regarding the suitability of the YMP in the SR is analogous to the burden of reasonable assurance that would be required if the YMP is recommended and a LA prepared for the NRC to review. Therefore, the suggestions received from the Peer Review Panel are equally germane to the TSPA-SR as they are to the eventual TSPA-LA (if the site is recommended).

This philosophy has been embraced in the methods and approach to the development of the TSPA-SR that is included in this document. Section 3 describes the current approach for implementing the individual component models into the TSPA-SR. In each section of Section 3, details are provided on the current approach that will be followed in the development of the TSPA-SR case. In addition, sensitivity analyses to evaluate the component models are described.

Any particular analysis will mix and match realistic and conservative assumptions. In fact, some components of the system may be so complex or intractable, that even the realistic reasonable representation includes some conservative bounding assumptions. This may be the case, for example, for radionuclide transport within a degraded waste package. The exact combination of realism and conservatism for each of the parameters and models will be clearly identified in each of the TSPA analyses.

1.3.4 The Safety Case for Total System Performance Assessment–Site Recommendation

The philosophy and approach to developing the case regarding postclosure safety is presented in the draft Repository Safety Strategy (DOE 1999). The postclosure safety case comprises the information DOE intends to use to assure a repository at Yucca Mountain would adequately protect public health and safety after the repository is permanently closed. This postclosure safety case will rest on a sound technical basis including information about the Yucca Mountain site, a robust design for the system, comprehensive safety assessments, and assessments of the confidence in that information.

The current version of the Repository Safety Strategy utilizes five lines of evidence to support the safety case:

- Performance Assessment
- Design margin and defense-in-depth
- Explicit consideration of potentially disruptive processes and events
- Insights from natural analogues
- Performance confirmation program.

The performance assessment of this safety case will focus on 27 factors for the nominal scenario and other factors for scenarios for disruptive processes and events. These factors are summarized in Table 1.3-1. Table 1.3-1 also shows the factors that were considered in the VA grouped according to the key attributes of the system as defined in the VA. From an analysis point of view, the factors identified in Table 1.3-1 represent groupings of FEPs containing the necessary and sufficient analyses and models to be used in the TSPA. The factors being developed to support the TSPA-SR are described more precisely (i.e., specific analyses, models, and parameters) in Section 3 of this document.[3]

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[3] Although the current version of the Repository Safety Strategy does not define factors for the scenarios for disruptive processes and events, the table refers to both nominal performance and disruptive processes and events. The focus of the analyses of potentially disruptive events for the SR will be on the volcanic and seismic/structural deformation processes and events. Potential criticality events will be analyzed and either screened in or out based on the scenario screening methodology presented in Section 2.2 of this document. Inadvertent human intrusion analyses, as required in the proposed 10 CFR 63 (64 FR 8640) will be constructed and documented in the TSPA-SR document.

Table 1.3-1. Comparison of Principal Factors of the Repository Safety Strategy Used in the VA With the Factors Used in the SR

Key Attributes of System	Principal Factors in VA[a]	Factors in Repository Safety Strategy Rev. 3[b]
Water Contacting Waste Package	Precipitation and Infiltration into the Mountain	Climate
		Infiltration
	Percolation to Depth	Unsaturated Zone (UZ) Flow Above Repository
	Seepage into Drifts	Seepage into Drifts *
	Effects of Heat and Excavation on Flow	Coupled Processes—Effects on UZ Flow
		Coupled Processes—Effects on Seepage
	N/A	Environments on Drip Shield
	N/A	Performance of Drip Shield *
Waste Package Lifetime	Dripping onto the Waste Package	Environments on Waste Package
	Humidity and Temperature at the Waste Package	
	Chemistry on the Waste Package	
	Integrity of Outer Waste Package Barrier	Performance of Waste Package Barriers *
	Integrity of Inner Waste Package Barrier	
Radionuclide Mobilization and Release From the EBS	Seepage into Waste Package	Environments Within Waste Package
	Integrity of SNF Cladding	Commercial Spent Nuclear Fuel (CSNF) Waste Form Performance
	Dissolution of UO_2 and Glass Waste Forms	DOE-Owned Spent Nuclear Fuel (DSNF), Navy Fuel, and Plutonium Disposition Waste Form Performance
		Defense HLW Glass Waste Form Performance
	Solubility of Neptunium-237	Solubility Limits of Dissolved Radionuclides*
	Formation of Radionuclide Bearing Colloids	Colloid Associated Radionuclide Concentrations
	Transport Within and Out of the Waste Package	In-Package Radionuclide Transport
	EBS Radionuclide Migration—Transport Through Invert	Transport Through Invert
Transport Away From the EBS	Transport Through UZ	Advective Pathways in the UZ
		Retardation of Radionuclide Migration in the UZ *
		Colloid Facilitated Transport in the UZ
		Coupled Processes—Effects on UZ Transport
	Transport in Saturated Zone (SZ)	Advective Pathways in the SZ
		Retardation of Radionuclide Migration in the SZ *
		Colloid Facilitated Transport in the SZ
	Dilution From Pumping	Dilution of Radionuclide Concentrations in the UZ and SZ *
	Biosphere Transport and Uptake	Biosphere Transport and Uptake
Effects of Potentially Disruptive Processes and Events	--	Factors for Igneous Activity Scenarios
		Factors for Seismic Activity Scenarios

[a] DOE 1998a.

[b] DOE 1999.

* Principal Factors in Revision 3 of Repository Safety Strategy (DOE 1999).

Of the 27 factors that need to be included in the nominal performance assessment, seven have been identified as principal factors of the safety case. The principal factors are those that have been determined, based on preliminary models and analyses, to most significantly impact the calculated postclosure performance. In addition to these analyses, limitations and uncertainties in the models and analyses were also considered in the development of the principal factors. The principal factors identified in Revision 3 of the Repository Safety Strategy (DOE 1999) include:

- Seepage into drifts
- Solubility limits of dissolved radionuclides
- Dilution of radionuclide concentrations in the UZ and SZ
- Retardation of radionuclide migration in the UZ
- Retardation of radionuclide migration in the SZ
- Performance of the drip shield
- Performance of the waste package barriers

The factors identified in the Repository Safety Strategy can be correlated with other means of combining the FEPs that have been used in other DOE and NRC documents. Tables 1.3-2 and 1.3-3 illustrate how the 27 factors of Revision 3 of the Repository Safety Strategy (DOE 1999), correlate with NRC subsystem components, key elements of subsystem abstraction (KESA), and key technical issues. Table 1.3-3 also shows a correlation of the factors with the Process Model Reports (PMR) that will contain a synthesis of the technical information used to support the representation of these factors in the TSPA-SR. The PMRs are analogous to the Technical Bases Documents (CRWMS M&O 1998a, Chapters 1 through 11) used to support the TSPA-VA. The PMRs will contain the necessary and sufficient information to defend the credibility of the TSPA-SR case. There will be nine PMRs and they are discussed in more detail in Section 1.5. The PMRs are, in turn, supported by a suite of Analysis and Model Reports (AMR). The principal AMRs supporting the TSPA-SR are tabulated in Table 1.3-4.

Although the technical basis for each factor is defined in the corresponding PMR listed in Table 1.3-3 and AMR listed in Table 1.3-4, the complete integration of the individual factors occurs within the context of the TSPA analyses. Sensitivity analyses of the key input variables affecting each factor will be documented in the PMRs and the supporting AMRs, but the integration of the various factors as they affect system and subsystem performance will be presented in the TSPA-SR document.

1.4 GENERAL APPROACH TO TOTAL SYSTEM PERFORMANCE ASSESSMENT–SITE RECOMMENDATION

In general, the goal of TSPA-SR is to provide decision makers with a reasonable estimate of the realistic future performance of the disposal system and a clear display of the extent to which uncertainty in the present understanding of the system affects that estimate. The results of TSPA-SR will be used to evaluate compliance with quantitative regulatory standards, taking uncertainty into account.

Table 1.3-2. Correlation of Relationship Among Repository Safety Strategy Factors, Subsystem Components, and KESA

Key Attributes of System	Factors[a]	NRC[b] Subsystem Components	NRC KESA[b]
Water Contacting Waste Package	Climate	UZ Flow and Transport	Spatial and Temporal Distribution of Flow
	Infiltration		
	UZ Flow Above Repository		
	Seepage into Drifts		
	Coupled Processes—Effects on UZ Flow		
	Coupled Processes—Effects on Seepage		
	Environment on Drip Shield	Engineered Barriers	Quantity and Chemistry of Water Contacting Waste Packages and Waste Forms
	Performance of Drip Shield		
Waste Package Lifetime	Environment on Waste Package		
	Performance of Waste Package Barriers		Waste Package Corrosion
			Mechanical Disruption of Waste Packages
Radionuclide Mobilization and Release from the EBS	Environment Within Waste Package		Radionuclide Release Rates and Solubility Limits
	CSNF Waste Form Performance		
	DSNF, Navy Fuel, Plutonium Disposition Waste Form Performance		
	HLW Glass Waste Form Performance		
	Solubility Limits of Dissolved Radionuclides		
	Colloid Associated Radionuclide Concentrations		
	In-Package Radionuclide Transport		
	Transport Through Invert		
Transport Away from the EBS	Advective Pathways in the UZ	UZ Flow and Transport	Distribution of Mass Flux Between Fracture and Matrix
	Retardation of Radionuclide Migration in the UZ		Retardation in Fractures in the UZ
	Colloid Facilitated Transport in the UZ		
	Coupled Processes—Effects on UZ Transport		
	Advective Pathways in the SZ	SZ Flow and Transport	Flow Rate in Water Productions Zones
	Retardation of radionuclide migration in the SZ		Retardation in Water Production Zones and Alluvium
	Colloid Facilitated Transport in the SZ		
	Dilution of Radionuclide Concentrations in the UZ and SZ	Dose Calculations	Dilution of Radionuclides in Groundwater
	Biosphere Transport and Uptake		Dilution of Radionuclides in Soil
			Lifestyle of Critical Group

Table 1.3-2. Correlation of Relationship Among Repository Safety Strategy Factors, Subsystem Components, and KESA (Continued)

Key Attributes of System	Factors[a]	NRC[b] Subsystem Components	NRC KESA[b]
Effects of Potentially Disruptive Processes and Events	Factors for Igneous Activity Scenarios	Direct Release and Transport	Volcanic Disruption of Waste Packages
			Airborne Transport of Radionuclides
	Factors for Seismic Activity Scenarios	Engineered Barriers	Mechanical Disruption of Waste Packages

[a] Factors From the Repository Safety Strategy (DOE 1999).

[b] Subsystem Components From the TSPA and Integration (TSPA&I) Key Technical Issue – Issue Resolution Status Report (IRSR) (NRC 1998a).

Table 1.3-3. Relationship Among the Repository Safety Strategy Factors, Key Technical Issues, and PMR

Key Attributes of System	Factors[a]	NRC[b] Key Technical Issue	Process Model Report
Water Contacting Waste Package	Climate	Unsaturated and Saturated Flow Under Isothermal Conditions	UZ Flow and Transport
	Infiltration		
	UZ Flow Above Repository		
	Seepage into Drifts	Repository Design and Thermomechanical Effects	
	Coupled Processes—Effects on UZ Flow	Thermal Effects on Flow	Near-Field Environment
	Coupled Processes—Effects on Seepage		
	Environment on Drip Shield	Evolution of the Near-Field Environment	EBS
	Performance of Drip Shield		Waste Package
Waste Package Lifetime	Environment on Waste Package		EBS
	Performance of Waste Package Barriers		Waste Package
Radionuclide Mobilization and Release From the EBS	Environment Within Waste Package	Container Life and Source Term	Waste Form
	CSNF Waste Form Performance		
	DSNF, Navy Fuel, Plutonium Disposition Waste Form Performance		
	HLW Glass Waste Form Performance		
	Solubility Limits of Dissolved Radionuclides		
	Colloid Associated Radionuclide Concentrations		
	In-Package Radionuclide Transport		
	Transport Through Invert		EBS
Transport Away From the EBS	Advective Pathways in the UZ	Radionuclide Transport	UZ Flow & Transport
	Retardation of Radionuclide Migration in the UZ		
	Colloid Facilitated Transport in the UZ		
	Coupled Processes—Effects on UZ Transport		
	Advective Pathways in the SZ		SZ Flow and Transport
	Retardation of Radionuclide Migration in the SZ		
	Colloid Facilitated Transport in the SZ		
	Dilution of Radionuclide Concentrations in the UZ and SZ		
	Biosphere Transport and Uptake		Biosphere

Table 1.3-3. Relationship Among the Repository Safety Strategy Factors, Key Technical Issues, and Process Model Reports (Continued)

Key Attributes of System	Factors[a]	NRC[b] Key Technical Issue	Process Model Report
Effects of Potentially Disruptive Processes and Events	Factors for Igneous Activity Scenarios	Igneous Activity	Tectonic Hazards
	Factors for Seismic Activity Scenarios	Structural Deformation and Seismicity	

[a] Factors From the Repository Safety Strategy (DOE 1999).

[b] Key Technical Issues from the TSPA&I Key Technical Issue – IRSR (NRC 1998a).

Table 1.3-4. Relationship Between the Repository Safety Strategy Factors and AMR That Provide Input to TSPA-SR

Key Attributes of System	Factors	Analysis and Model Report Number	Analysis and Model Report Title
Water Contacting Waste Package	Climate	U0005	Climate Model Abstraction
	Infiltration	U0095	Infiltration Uncertainty Abstraction
	UZ Flow Above Repository	U0125	UZ Flow Fields Abstraction
	Seepage into Drifts	U0120	Drift Seepage and Coupled Process Abstraction
	Coupled Processes—Effects on UZ Flow	U0115	UZ Coupled Process Flow Field Abstraction
	Coupled Processes—Effects on Seepage	U0120	Drift Seepage and Coupled Process Abstraction
	Environment on Drip Shield	N0065	Near-Field Thermodynamic Environment Abstraction
		E0010	EBS Physical Chemical Environment Abstraction
		E0090	EBS Water Distribution and Removal Model
	Performance of Drip Shield	W0075	Juvenile Failures
		W0125	Abstraction of Model for Mechanical Damage and Failure of Drip Shield and Waste Package by Rockfall
		W0005	Abstraction of Models for General Corrosion of Drip Shield and Waste Package Outer Barrier
		W0040	Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier
		W0045	Abstraction of Models for Stress Corrosion Cracking (SCC) of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Cracking (HIC) of Drip Shield
		W0030	Failures Due to Mechanical Degradation

Table 1.3-4. Relationship Between the Repository Safety Strategy Factors and AMR That Provide Input to TSPA-SR (Continued)

Key Attributes of System	Factors	Analysis and Model Report Number	Analysis and Model Report Title
Waste Package Lifetime	Environment on Waste Package	E0010	EBS Physical Chemical Environment Abstraction
		N0065	Near-Field Thermodynamic Environment Abstraction
		E0090	EBS Water Distribution and Removal Model
	Performance of Waste Package Barriers	W0075	Juvenile Failures
		W0020	Aging and Phase Stability of Waste package Outer Barrier
		W0125	Abstraction of Model for Mechanical Damage and Failure of Drip Shield and Waste Package by Rockfall
		W0005	Abstraction of Models for General Corrosion of Drip Shield and Waste Package Outer Barrier
		W0040	Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier
		W0045	Abstraction of Models for SCC of Drip Shield and Waste Package Outer Barrier and HIC of Drip Shield
		W0120	Abstraction of Models for Stainless Steel Structural Material Degradation
Radionuclide Mobilization and Release From the EBS	Environment Within Waste Package	F0135	In-Waste Package Temperature History
		F0130	In-Waste Package Chemistry History
		F0165	In-Waste Package Hydrology History
	CSNF Waste Form Performance	F0015	CSNF Inventory Abstraction
		F0155	Cladding Degradation Abstraction
		F0055	CSNF Degradation Model
	DSNF, Navy Fuel, Plutonium Disposition Waste Form Performance	F0015	DSNF Inventory Abstraction
		F0065	Other Waste Form Degradation Abstraction
	HLW Glass Waste Form Performance	F0015	HLW Inventory Abstraction
		F0060	HLW Glass Degradation
	Solubility Limits of Dissolved Radionuclides	F0095	Dissolved Concentration Limits Abstraction
	Colloid Associated Radionuclide Concentrations	F0115	Colloid Source Term Abstraction
	In-Package Radionuclide Transport	F0165	In-Waste Package Hydrology History
	Transport Through Invert	N0065	Near-Field Thermodynamic Environment Abstraction
		E0095	EBS Radionuclide Transport Abstraction

Table 1.3-4. Relationship Between the Repository Safety Strategy Factors and Analysis and Model Reports that Provide Input to TSPA-SR (Continued)

Key Attributes of System	Factors	Analysis and Model Report Number	Analysis and Model Report Title
Transport Away From the EBS	Advective Pathways in the UZ	U0125	UZ Flow Fields Abstraction
	Retardation of Radionuclide Migration in the UZ	U0065	UZ Transport Particle Tracking Abstraction
		U0100	UZ/SZ Transport Properties
	Colloid Facilitated Transport in the UZ	U0070	UZ Colloid Transport Model
	Coupled Processes—Effects on UZ Transport	U0100	UZ/SZ Transport Properties
	Advective Pathways in the SZ	S0055	SZ Flow and Transport Model Abstraction
		S0050	SZ Flow and Transport Stochastic Parameters
	Retardation of Radionuclide Migration in the SZ	S0050	SZ Flow and Transport Stochastic Parameters
		U0100	UZ/SZ Transport Properties
	Colloid Facilitated Transport in the SZ	S0035	Colloid Facilitated Transport
	Dilution of Radionuclide Concentrations in the UZ and SZ	B0015	Water Usage
		B0010	Critical Group
	Biosphere Transport and Uptake	B0075	Biosphere Dose Conversion Factors (BDCF)
Effects of Potentially Disruptive Processes and Disruptive Events	Factors for Igneous Activity Scenarios	T0015	Framework for Igneous Activity
		T0070	Consequence Analysis of Direct Release
	Factors for Seismic Activity Scenarios	T0075	Framework for Seismicity/Structural
		T0110	Consequence Analysis Result

Because regulatory requirements ask for an estimate of the expected (or mean) annual dose and a consideration of the uncertainty in that estimate, the Yucca Mountain TSPA uses a probabilistic approach similar to that adopted by many other repository programs internationally. This approach has five major steps, briefly summarized below.

Develop and Screen Scenarios–The first step in the TSPA is to decide what representations of possible future states of the repository, or scenarios, are sufficiently important to warrant quantitative analysis. Further definition of scenarios is found in Appendix A. TSPAs can analyze only a relatively small number of the essentially infinite combinations of processes and events that could conceivably affect the system. The chosen scenarios shall be representative of the conditions of greatest relevance to regulatory requirements and the long-term safety of the site. Estimates shall be provided of the probability that the chosen scenarios will occur. The scenario development process documents the basis for scenario selection and screening.

Develop Models–In this step, models are developed to represent components of the system that are potentially important in the chosen scenarios. These models are first developed as conceptual models that describe the behavior of the system. Mathematical models are developed that quantify the conceptual models, and then, in most cases, the mathematical models are implemented in computer codes. The developed models, used to describe the individual components of the TSPA-SR model, will be documented in a series of AMRs and synthesized into the nine PMRs discussed in Section 1.5.

Estimate Parameter Ranges and Uncertainties–Many parameters used in the TSPA models (e.g., those that describe common rock properties like porosity and permeability) have natural variability. Uncertainty regarding parameter values also arises from incomplete knowledge (e.g., when the future state of a property must be estimated from assumptions rather than from measurements). Uncertainty associated with the selection of parameter values for the TSPA is accounted for by developing distributions of values for important, and imprecisely known, parameters rather than using single values. Each distribution describes a range of values within which the true value is believed to fall, with an expected value (i.e., the mean) that corresponds to the best estimate of the true value. Not all parameters in the TSPA require uncertainty distributions. Single values are used to describe properties that are well-known, or for which uncertainty has been shown to have little or no effect on overall performance.

Perform Calculations–Computer models are linked to allow calculation of the overall system behavior. Uncertainty associated with the selection of scenarios is included in the TSPA by conducting separate analyses for each scenario. Uncertainty associated with the model parameters is included in the TSPA by conducting multiple calculations for each scenario using values sampled from the ranges of possible values. Each individual calculation uses a different set of sampled input values. In a statistical sense, the result of each individual TSPA calculation represents a different possible realization of the future performance of the system, consistent with the uncertainty in the input parameters. The expected (i.e., mean) behavior of the system for each scenario is shown by the mean of the results of the individual calculations, and the uncertainty associated with that mean is shown by the range of calculated outcomes. The overall expected annual dose estimate required by proposed 10 CFR 63 (64 FR 8640) is determined by summing the expected annual dose calculated for each scenario, weighted by the probability that the scenario will occur. The TSPA is, therefore, a probabilistic analysis consistent with the requirements of proposed 10 CFR 63 (64 FR 8640) as described in Section 2, in the sense that it takes into account both the estimates of the probability of occurrence of the different scenarios and the uncertainty associated with input parameters.

Interpret Results–Results of preliminary performance assessments can be analyzed at the system and subsystem levels to identify the models and parameters that have the greatest effect on the behavior of the system. Identification of the uncertainties that are most important to the TSPA can help guide future testing for site characterization, model development, and repository design. When the TSPA models are sufficiently well developed and documented to support regulatory decisions, results can be used to evaluate compliance with applicable long-term requirements.

1.5 PLANNED DOCUMENTS TO SUPPORT THE TOTAL SYSTEM PERFORMANCE ASSESSMENT–SITE RECOMMENDATION

The TSPA-SR analyses will be built upon a significant body of scientific and engineering data, analyses, and models. The technical bases for the models used to predict the postclosure performance will be described within the previously mentioned family of documents called PMRs. As noted, these documents are analogous to the Technical Basis Documents prepared to support the TSPA-VA. The nine PMRs planned to support the TSPA-SR are:

- Integrated Site Model

- UZ Flow and Transport Model
- Near-Field Environment Model
- EBS Degradation, Flow and Transport Model
- Waste package Degradation Model
- Waste Form Degradation Model
- SZ Flow and Transport Model
- Biosphere Transport Model
- Tectonic Hazards Models.

These PMRs, which will synthesize the scientific information available to support the models used in the TSPA-SR analyses, are in turn built upon a set of AMRs, which in turn, are derived from site and laboratory data and other information sources.

The flow of information and the hierarchy of technical documents that support the major programmatic milestones of the Final EIS, the Considerations Hearings, and the SR are illustrated in Figure 1.5-1. This figure illustrates the various revisions of the TSPA analyses (i.e., the TSPA-SR Revision 00, TSPA-SR Revision 01 and TSPA-LA), and shows the revisions of the PMRs that will support the TSPA revisions.

The TSPA documentation will be developed as three separate, evolving documents: TSPA-SR, Revision 00; TSPA-SR, Revision 01; and the TSPA chapter in the LA. The approach involves developing the initial Revision 00, followed by revisions at two separate points in time to provide the updated analysis and focus on specific requirements in the subsequent documents.

The TSPA-SR, Revision 00, will primarily consist of discussion of the expected performance case as defined in the proposed 10 CFR 63 (64 FR 8640). The document will have extensive discussion of the analyses and how they provide reasonable assurance of the performance of the repository system. Because the technical details providing the basis for the models used in the TSPA analyses will be contained within the PMRs and supporting AMRs, the TSPA-SR documentation itself will focus on how the individual component models were combined in the TSPA and will provide enough subsystem analysis to illustrate how the overall system is projected to perform. Sensitivity analyses will be included in Revision 00. While proposed sensitivity analyses are described in this document, the details of the sensitivity analyses will be worked out in the coming months.

The TSPA-SR, Revision 01, will be an update of the TSPA-SR, Revision 00. There will not be major changes in the overall modeling and analysis structure from Revision 00 to Revision 01, given the short amount of time between the versions. This revision will primarily address comments received from the public and oversight bodies on the Revision 00 analyses.

The TSPA-LA will be a chapter in the LA. However, it is envisioned to be an update of TSPA-SR, Revision 01. A primary addition from the previous version will be the inclusion of an evaluation of each of the relevant NRC key technical issues and the IRSR acceptance criteria. This revision will be formatted to be consistent with the NRCs Yucca Mountain Review Plan and address particular regulatory issues.

1.6 ORGANIZATION OF THIS DOCUMENT

Following the introductory information presented in Section 1, three other sections are presented that contain descriptions of the overall completeness of the TSPA (Section 2), the components of the TSPA model (Section 3), and the TSPA structure and analyses (Section 4). References are provided in Section 5. The specific content of each section is summarized in the following paragraphs:

Section 2: Completeness of the TSPA–The TSPA approach to the definition and disposition of FEPs is detailed in this section, showing how the analyses are complete in their consideration of the appropriate FEPs. Additionally, the section provides information on the approach taken in the analyses to respond to NRC IRSRs (NRC 1997a through 1997e; NRC 1998a through 1998e). the Performance Assessment Peer Review (PAPR) panel comments (Whipple et al. 1997a; 1997b; 1998; 1999), and other issues identified by oversight agencies. Finally, the section describes the software QA and configuration management utilized in the TSPA modeling and aspects of transparency and traceability.

Section 3: Components of the TSPA–The approach to the analysis of each of the major components of the TSPA is presented in this section of the document. The overall TSPA model and code architecture is described. The components include UZ flow and transport, thermohydrology and coupled processes, in-drift geochemical environment (IDGE), waste package and drip shield degradation, waste form degradation, EBS transport, SZ flow and transport, and biosphere. In addition, the section discusses disruptive event scenarios separately. Each of the subsections provides information on general description of the process model and abstraction, major assumptions in the analyses, description of the TSPA-SR conceptual model and possible sensitivity cases, and any significant coupling with other components. The issue of conservatism in the models is also discussed briefly. The assumptions are listed and will be tracked in the SR documentation. The analyses discussed in this section are expected to be conducted for TSPA-SR, however, they may be changed prior to completion of TSPA-SR due to findings from the AMR's or scheduling issues.

Section 4: TSPA Analyses–The approach to the analyses required for SR, is the main aspect described in this section. The approach to nominal scenarios, disruptive scenarios, and combined analyses is presented. Additionally, the method for uncertainty and sensitivity analyses will be described. The multiple barrier analyses important to evaluation of robust performance are also considered in this section. A small selection of alternative designs may be analyzed in the TSPA-SR, and this is described in the section. The discussion of human intrusion analyses and consequence analyses close the section.

Section 5: References–A listing of the references utilized in the document is provided. The appropriate accession number is identified for all documents referenced.

Appendix A: Glossary–A brief listing of key words used in the document is presented in this appendix.

This document defines the approach for TSPA-SR as it is currently envisioned. Changes to this approach may be required due to technical exchanges with the NRC, final promulgation of proposed 10 CFR 63 (64 FR 8640), final promulgation of 40 CFR 197, and technical development of the TSPA-SR. This document, therefore, summarizes the general approach and methodology. The detailed implementation of this approach and methodology will occur over the coming months and will utilize a suite of process models, abstraction models, and supporting technical analyses contained within individual AMRs.

1.7 APPLICABILITY OF QUALITY ASSURANCE PROGRAM

The QA program applies to the development of this report. The Performance Assessment Operations (PAO) responsible manager has evaluated the technical document development activity in accordance with QAP-2-0, *Conduct of Activities*. The QAP-2-0 activity evaluation. *Activity Evaluation for Conduct of Performance Assessment* (CRWMS M&O 1999b), has determined that the preparation and review of this technical document is subject to *Quality Assurance Requirements and Description* (DOE 1998d) requirements. In accordance with AP-3.11Q, *Technical Reports*, and AP-2.13Q, *Technical Product Development Planning*, a development plan was developed, issued, and utilized in the preparation of this document (CRWMS M&O 1999c).

Since the purpose of this document is to present the methods and approach to be used for the development of the TSPA-SR, the technical product inputs do not require tracking as to be verified/to be determined (TBV/TBD). This is in accordance with Section 5.2.1 (i) and Attachment 3 of AP-3.15Q, *Managing Technical Product Inputs*. The Attachment 3 determination concluded that the inputs, with respect to this report, will not affect a system's critical characteristics, scientific results or conclusions, and will not be directly relied upon to address safety or waste isolation issues.

2. REGULATORY AND COMPLETENESS ISSUES OF CONCERN TO TOTAL SYSTEM PERFORMANCE ASSESSMENT

The TSPA-SR will play a pivotal role in the DOE and Presidential decision making processes, and the analyses and documentation must be complete in regulatory and technical aspects. The primary regulation governing the SR is the DOE's 10 CFR 963 (pending), which will be consistent with the NRC's proposed 10 CFR 63 (64 FR 8640). The NRC's proposed rule in turn establishes criteria implementing the EPA's proposed 40 CFR 197. Completeness of the SR with respect to regulatory issues will be judged by criteria established in 10 CFR 963: however, relevant criteria established in the NRC and EPA regulations will also be considered in the design of the TSPA-SR. In addition, completeness of the technical aspects of the TSPA will be addressed through careful consideration of technical guidance provided by the NRC through their TSPA&I IRSR (NRC, 1998a) and other comments and recommendations from regulatory, oversight, and peer review groups.

Section 2 contains six subsections related to regulatory and completeness issues. Section 2.1 summarizes key aspects of the 10 CFR 963 and other relevant regulations. Section 2.2 describes the approach to demonstrating the completeness of the scenarios considered in the TSPA-SR, consistent with the NRC's requirement in proposed 10 CFR 63 (64 FR 8640) to "identify the features, events, and processes that might affect the performance of the geologic repository." Section 2.3 describes the status of the resolution of key technical issues raised by the NRC staff in their review of the YMP. Section 2.4 describes the comments of the Performance Assessment Peer Review (PAPR) Panel, which has provided an independent assessment of the completeness and adequacy of the TSPA. Section 2.5 discusses software quality assurance and configuration management, which are essential components of the DOE's strategy for ensuring the regulatory completeness of the SR. Section 2.6 discusses the approach to providing transparency and traceability in the TSPA-SR analyses.

2.1 REGULATORY REQUIREMENTS

The federal regulations applicable to the geologic disposal of HLW at Yucca Mountain, Nevada, will ultimately prescribe how a performance assessment is to be conducted and documented, as well as the sufficiency of data needed to support the assessment. At present, the regulatory framework for a potential repository at Yucca Mountain is evolving. In the midst of this changing environment, personnel responsible for conducting the performance assessment will track the development of new regulations in order to be fully aware of the requirements that need to be addressed in the TSPA-SR.

With passage of the Energy Policy Act of 1992, Congress mandated that the EPA promulgate a standard specific to a potential repository at the Yucca Mountain site. In addition, Congress required the EPA to contract with the National Academy of Sciences (NAS) to study whether a dose standard is appropriate and to study two other issues related to institutional controls and human intrusion. The EPA standards were to be promulgated within one year of the receipt of the NAS study, with the implicit understanding that the EPA would give consideration to the findings and recommendations of the NAS. In 1995, the NAS released its study by publishing the *Technical Bases for Yucca Mountain Standards* (NAS/NRC 1995).

2.1.1 10 CFR 960

In accordance with the Nuclear Waste Policy Act of 1982, the DOE promulgated the regulation 10 CFR 960 in the mid-1980s for the purpose of establishing general guidelines for the recommendation of sites for nuclear waste repositories. The original siting guidelines set forth in the DOE regulation were intended to complement the then applicable NRC regulation 10 CFR 60 and EPA standard 40 CFR191.

The 10 CFR 960 regulation, for the most part, sets generic criteria for siting a repository in terms of the physical characteristics of a potential site and the surrounding area. In addition, it also contains an appendix that specifies postclosure performance criteria for a repository in terms of compliance with the total system requirement in the EPA standard 40 CFR 191 and subsystem requirements of the NRC regulation 10 CFR 60. Specifically, Appendix I entitled, "NRC and EPA Requirements for Postclosure Repository Performance," requires a demonstration of compliance with the containment requirements of 40 CFR 191; the containment requirements set limits in a probabilistic manner on the cumulative normalized radionuclide releases to the accessible environment for 10,000 years.

The 40 CFR 191, which was remanded by the courts, will be replaced by a new site-specific EPA standard, 40 CFR 197. Similarly, the 10 CFR 60 regulation is being replaced by a new NRC regulation, proposed 10 CFR 63 (64 FR 8640). As a result of these changes in the federal regulations, the DOE is examining options for revising the siting guidelines to ensure full consistency with these new regulations and anticipated standard.

Based on guidance from the DOE, TSPA-SR will incorporate the applicable regulatory requirements which are currently in proposed regulation 10 CFR 63 (Dyer 1999). However, if DOE siting guidelines are revised, personnel responsible for conducting the TSPA will identify and apply the new requirements.

2.1.2 Promulgation of Proposed 10 CFR 63 (64 FR 8640)

In the absence of 10 CFR 963, the TSPA-SR is focused on addressing the performance requirements contained in the NRC proposed 10 CFR 63 (64 FR 8640). The NRC has undertaken development of the implementing regulations ahead of the promulgation of the EPA environmental radiation protection standards. The proposed NRC rule has been published in the Federal Register. Personnel responsible for conducting the performance assessment are reviewing and evaluating the proposed 10 CFR 63 (64 FR 8640) for requirements related to how to conduct a TSPA, and will highlight the differences between the requirements of 10 CFR 60 and the proposed 10 CFR 63 (64 FR 8640). For some new requirements, as with the consideration of human intrusion, planning already is underway to determine how to incorporate the requirements into the TSPA-SR. When the proposed rule becomes final, personnel responsible for conducting the performance assessment will review the rule and identify any changes from the proposed rule. At that time, all additional changes to the TSPA methodology will be made.

2.1.3 Promulgation of 40 CFR 197

Concurrent with the NRC rulemaking process, the EPA is currently developing Yucca Mountain specific standards, designated as 40 CFR 197. As with the development of proposed 10 CFR 63 (64 FR 8640), personnel responsible for conducting the performance assessment will review the proposed and final versions of 40 CFR 197 when they are published in the Federal Register to understand the performance assessment requirements. Upon the promulgation of 40 CFR 197, personnel responsible for conducting the performance assessment will identify any differences between it and proposed 10 CFR 63 (64 FR 8640), evaluate means of complying with both sets of requirements (if possible), and participate (as appropriate) in efforts to reconcile the differences.

2.1.4 Potential Repromulgation of Proposed 10 CFR 63 (64 FR 8640)

The Energy Policy Act of 1992 mandates that the NRC modify its implementing regulation to be consistent with the public health and safety standards developed by the EPA for Yucca Mountain. Consistency between EPA standards and NRC technical requirements and criteria must be established within one year after the promulgation of EPA standards. Personnel responsible for conducting the performance assessment will evaluate any repromulgation of proposed 10 CFR 63 (64 FR 8640) to determine if there are any changes in performance assessment requirements. If changes are required, they will be implemented in the next TSPA analysis.

2.2 THE FEATURES, EVENTS, AND PROCESSES APPROACH

Scenario development has two primary purposes in the design and documentation of postclosure performance assessments in a regulatory setting. First, scenario development ensures a sufficiently comprehensive consideration of the possible future states of the repository system. Second, scenario development identifies the important scenarios that must be considered in the TSPA. The approach is being used to satisfy requirements in proposed 10 CFR 63.

To ensure clear documentation of the treatment of potentially relevant future states of the system, the DOE has chosen to adopt a scenario development process based on the methodology developed by the NRC (Cranwell et al. 1990, Section 2.0). Although the process described below has been modified somewhat as a result of experience gained in the last decade, the underlying methodology is consistent with that outlined by the DOE in the 1988 *Site Characterization Plan: Yucca Mountain Site, Nevada Research and Development Area* (DOE 1988, Section 8.3.5). The approach is fundamentally the same as that used in many performance assessments, including the most recent analysis of the Yucca Mountain repository by the NRC (NRC 1995a, Chapter 3). The approach has also been used by the DOE for the Waste Isolation Pilot Plant (WIPP) (DOE 1996, Section 6.2), by the Nuclear Energy Agency (NEA) of the Organization for Economic Co-Operation and Development (NEA 1992), and by other radioactive waste programs internationally (e.g., Skagius and Wingefors 1992, Section 2).

The five principal steps in the scenario development process are illustrated in Figure 2.2-1, discussed in detail in the following sections, and outlined below:

1. Identify and classify FEPs potentially relevant to the long-term performance of the disposal system.

2. Screen the FEPs using well-defined criteria to distinguish between those FEPs that can be excluded from the TSPA and those that should be included in the analysis.

3. Use the retained FEPs to construct scenarios, or scenario classes (which are defined as sets of related scenarios), as appropriate.

4. Screen the scenarios (or scenario classes) using the same criteria applied to the FEPs to identify any scenarios that can be excluded from the TSPA.

5. Specify the implementation of the scenarios (or scenario classes) in the computational modeling for the TSPA, and document the treatment of included FEPs.

These five steps differ slightly from those identified by the NRC (Cranwell et al. 1990, Section 2.0), in that FEP classification, which was the second step in the NRC procedure, has been included with the first step. The final step has been modified to clarify the linkage between scenario development and the TSPA analysis. These steps are also slightly different from the steps outlined in the NRC's TSPA&I (NRC 1998a). Step 1 (identification of initial list of FEPs) and Step 2 (classification of the FEPs) from Subissue 4 of the IRSR have been combined in the TSPA-SR procedure. Again, the final step in this procedure goes beyond the IRSR requirements and links scenario development and the TSPA-SR analysis.

Step 1: Identification and Classification of FEPs–Step 1 of the scenario development process, the identification and classification of FEPs potentially relevant to the performance of the Yucca Mountain repository, addresses the first of these three requirements for a performance assessment as defined by the NRC at proposed 10 CFR 63.2 (64 FR 8640) (see Section 1.3.1).

The initial set of FEPs has been created for the Yucca Mountain TSPA by combining lists of FEPs previously identified as relevant to the YMP (e.g., by Wilson et al. 1994, Section 3.2; CRWMS M&O 1995, Section 2.7) with a draft FEP list compiled by an NEA working group. The NEA list is the most comprehensive list available internationally, and currently contains 1,261 entries from Canadian, Swiss, and Swedish spent fuel programs, intermediate and low-level waste programs of the United Kingdom, and the U.S. WIPP program.

FEPs are classified for the Yucca Mountain scenario development using the same structure adopted by the NEA. Many classification schemes are possible, and there is no inherently correct way to order FEPs. The DOE has chosen to adopt the NEA classification scheme without modification, because it maintains consistency between NEA and YMP databases, which facilitates reviewing for completeness.

The YMP FEP list currently contains more than 1,700 entries. The YMP FEP list will be available in electronic form at the time of the TSPA-SR. A discussion of the classification scheme used to organize the list will be provided in the introduction to the database.

The FEP list is open and may continue to grow if additional FEPs are identified during planning for the TSPAs that will support the SR and LA. Because one of the major goals of the process is to address the comprehensiveness of the TSPA, no FEPs are removed from the list at this stage. Consistent with the diverse backgrounds of the waste disposal programs contributing to the NEA list, FEPs currently on the list were identified by a variety of methods, including expert judgment, informal elicitation, event tree analysis, stakeholder review, and regulatory stipulation. For the purposes of the Yucca Mountain scenario development effort, no specific technique is identified as a preferred method of FEP identification. All potentially relevant FEPs are included, regardless of origin.

This approach leads to considerable redundancy in the FEP list, because the same FEPs are frequently identified by multiple sources. To eliminate this redundancy and to create a more useful FEP list to carry forward into the screening process in Step 2, FEPs are further classified in this step as either primary FEPs or secondary FEPs. Primary FEPs are those for which the YMP proposes to develop detailed screening arguments. Secondary FEPs are either FEPs that are completely redundant (e.g., the NEA list contains as many entries for meteorite impact as there were participating programs), or FEPs that can be aggregated into a single primary FEP for the purposes of the Yucca Mountain TSPA. Examples of secondary FEPs that can be aggregated into a single primary FEP for Yucca Mountain include almost all FEPs related to the mode of human disruption of the disposal system, given the proposed regulatory requirement regarding the treatment of human intrusion through a prescribed drilling scenario.

FEPs that are unarguably irrelevant to the Yucca Mountain system, such as those specific to repositories in salt host rock, are also identified at this stage and are not carried through into Step 2 for the development of specific screening arguments.

Documentation will be provided of all mapping of FEPs into the primary and secondary categories and of any FEPs identified as irrelevant. Screening work in Step 2 focuses on the primary FEPs. For comprehensiveness, traceability is maintained from the secondary FEPs to the related primary FEPs.

Step 2: Screening of FEPs–Each FEP is screened for inclusion or exclusion in the TSPA on the basis of three basic criteria, developed from the requirements of proposed 10 CFR 63 (64 FR 8640). First, each FEP is examined to determine whether or not it is of regulatory concern, given the specific regulatory requirements applicable to the Yucca Mountain TSPA. For example, FEPs related to speculation about future human behavior are excluded from the analysis based on the specification of proposed 10 CFR 63.115 of assumptions about the critical group to be considered in the dose assessment (64 FR 8640). If the FEP is potentially of concern, it is then screened on the basis of its probability of occurrence or of its consequence.

The probability criterion is explicitly stated at proposed 10 CFR 63.114(d) (64 FR 8640):

> (d) Consider only events that have at least one chance in 10,000 of occurring over 10,000 years.

Because the probability of any specific event depends strongly on how it is defined, the probability criterion can only be applied at an appropriately broad scale. For example, the probability of seismic events should be evaluated over the entire 10,000-year period, rather than being artificially lowered by defining 10,000 different seismic events each occurring in a different year.

Consequence criteria are provided at proposed 10 CFR 63.114(e) and 63.114(f) (64 FR 8640):

> (e) Provide the technical basis for either inclusion or exclusion of specific features, events and processes of the geologic setting in the performance assessment. Specific features, events and processes of the geologic setting must be evaluated in detail if the magnitude and time of the resulting expected annual dose would be significantly changed by their omission.
>
> (f) Provide the technical basis for either inclusion or exclusion of degradation, deterioration, or alteration processes of engineered barriers in the performance assessment, including those processes that would adversely affect the performance of natural barriers. Degradation, deterioration, or alteration processes of engineered barriers must be evaluated in detail if the magnitude and time of the resulting expected annual dose would be significantly changed by their omission.

Because the regulatory requirements allow exclusion of FEPs on either low probability or low consequence, a FEP need not be shown to be both of low probability and low consequence to be excluded. Therefore, the order in which the criteria are applied is not essential.

In practice, FEPs are screened as shown in Figure 2.2-2. Regulatory criteria are examined first, and then either probability or consequence may be examined next at the discretion of the analyst. This application of the analyst's judgment regarding the order in which to apply the criteria does not affect the final decision. FEPs that are retained on one criterion will then be considered against the other. Needless work developing quantitative probability arguments for low consequence events or complex consequence models for low probability events is prevented by allowing the analyst to choose the most appropriate criteria to apply at this step (e.g., there is no need to develop detailed models of the response of the disposal system to the impact of a large meteorite if it can be shown that this event has a probability below the regulatory cutoff).

Probability estimates for FEPs may be based on technical analysis of the past frequency of similar events (e.g., seismic events) or, in some cases, on expert elicitation. Probability arguments, in general, require including some information about the magnitude of the event in its definition (e.g., the probability of meteorite impacts depends on the size of the meteorite of interest). Impacts of meteorites sufficiently large to create large craters at Yucca Mountain are much less probable than smaller impacts. Thus, meteorites large enough to affect the disposal system are screened out on the basis of low probability, but small impacts that have no effect are more appropriately screened out on low consequence. Probability arguments are also sensitive to the spatial and temporal scales at which FEPs are defined (meteorite impacts are less likely in shorter time intervals and at smaller locations), and probability arguments are therefore made at reasonably coarse scales.

The quantitative basis for consequence based screening arguments can be established in a variety of ways, including TSPA sensitivity analyses, modeling studies outside of the TSPA, or, in the case of relatively straightforward arguments, through the use of reasoned arguments based on literature research (e.g., consequences of many geomorphic processes, such as erosion and sedimentation, can be evaluated by considering bounding rates reported in geologic literature). More complicated processes, such as criticality, require detailed analyses conducted specifically for the YMP. Low-consequence arguments can be made by demonstrating that a particular FEP has no effect on the distribution of an intermediate performance measure in the TSPA (e.g., demonstrating that including a particular waste form has no effect on the concentrations of radionuclides transported from the repository in the aqueous phase may be sufficient to demonstrate that including this waste form would not change the expected annual dose). Explicit modeling of the characteristics of this waste form could therefore be excluded from the TSPA.

Documentation of the FEP screening step in the scenario development process provided in the FEP database will include a statement of the screening decision for each FEP (retained or excluded). For excluded FEPs, documentation will also include the criterion on which it was excluded and the technical basis for the screening argument. For retained FEPs, the FEP database contains a summary cross-reference to the discussion elsewhere in the supporting documentation of their treatment in the TSPA models and parameters.

Step 3: Constructing Scenarios from the Retained FEPs–The NRC does not define the term scenario in proposed 10 CFR 63 (64 FR 8640). The DOE has chosen to define a scenario for the Yucca Mountain TSPA as a subset of the set of all possible futures of the disposal system that contains futures resulting from a specific combination of FEPs.

The primary reason for adopting this definition is pragmatic. One of the goals of scenario development is to define a limited set of scenarios that can reasonably be analyzed quantitatively while still maintaining comprehensive coverage of the range of possible future states of the system. There are an essentially infinite number of possible future states, and for scenario development to be useful, it must generate scenarios that are representative of the range of futures that are potentially relevant to the licensing of the facility.

Under the definition adopted for the Yucca Mountain TSPA, a scenario is not limited to a single, deterministic future of the system; instead, it is a set of similar futures that share common FEPs. The number and breadth of scenarios depend on the resolution at which the FEPs have been defined. Coarsely defined FEPs result in fewer, broad scenarios, whereas narrowly defined FEPs result in many narrow scenarios. There is no correct level of detail that defines scenarios. Decisions regarding the appropriate level of resolution for the analysis are made based on consideration of the importance of the scenario in its effect on overall performance and the resolution desired in the results. For efficiency, FEPs and scenarios should be aggregated at the coarsest level at which a technically sound argument can be made that is adequate for the purposes of the analysis.

More coarsely defined scenarios may be referred to as scenario classes (sets of closely related scenarios), and more narrowly defined scenarios may be referred to as subscenarios. Mathematically, scenario classes and subscenarios share the same definition as scenarios (all are subsets of the set of all possible futures of the system). In practical application, however, distinguishing between coarsely defined scenario classes and more narrowly defined scenarios and subscenarios is useful (e.g., both the DOE and the NRC have identified "igneous activity occurs at Yucca Mountain" as one of the most important disruptive scenario classes for the repository). Within this class, consequence analyses have focused on specific scenarios and subscenarios involving processes such as ash plume eruption and magma intrusion.

Before scenarios are constructed, FEPs retained from Step 2 are identified as either expected FEPs (EFEPs) or disruptive FEPs (DFEPs). EFEPs are those that can be assumed, for the purposes of the TSPA, to have a probability of occurrence equal to 1.0 (although they may have uncertain consequences). DFEPs are those that have a probability less than 1.0 (but greater than the lower cutoff prescribed by the NRC) and have a significant effect on overall performance. All EFEPs are included in a nominal scenario, which is simulated by the base case model described in the TSPA documentation. Disruptive scenarios are constructed from all EFEPs and combinations of DFEPs, with the probability of each disruptive scenario calculated as the product of the probabilities of the included DFEPs.

Scenario construction can be displayed graphically using logic diagrams (Figure 2.2-3). Note that these diagrams do not imply any ordering of the events. They are simply a graphical way of displaying the possible combinations of the retained DFEPs. Mathematically, they are interchangeable with the Latin Square approach (Figure 2.2-4) used by the NRC to display combinations of retained disruptive events in the TSPA&I (NRC 1998a, Rev. 1, Section 4.4.5). Using either logic diagrams or Latin Squares, scenario probabilities are calculated simply as the product of the probability of the occurrence and nonoccurrence of each FEP used in building the scenario.

Step 4: Screening Scenarios–Scenarios constructed in Step 3 are screened using the same regulatory, probability, and consequence criteria defined in Step 2. For example, the probability criterion may be used to exclude scenarios that include some combinations of low probability FEPs.

If scenarios are to be screened out on the basis of low probability, the probability must be taken at an appropriately coarse level. Scenarios should not be defined artificially narrow to reduce their probability below the NRC cutoff.

Step 5: Implementing Scenarios in the TSPA–All retained FEPs must be included in TSPA analyses, either in the nominal scenario or in disruptive scenarios. EFEPs may be included in the nominal scenario, either through explicit modeling or through the selection of parameter values. DFEPs are included explicitly in modeling of disruptive scenarios.

As shown in Figure 2.2-2, retained FEPs are treated either through explicit incorporation in TSPA models or through uncertainty included in the assignment of parameter values used in the TSPA models. The FEP database will provide a summary statement of how each retained FEP has been addressed in the TSPA, as well as a cross-reference to the documentation of the appropriate models or data in the LA.

2.3 U.S. NUCLEAR REGULATORY COMMISSION ISSUE RESOLUTION STATUS REPORTS

The NRC staff has prepared a set of IRSRs to provide early and directed feedback to DOE regarding potential licensing vulnerabilities in the areas of postclosure performance assessment methodology, site characterization activities, and repository system engineered barrier design. The NRC staff has written ten IRSRs that are in various stages of finalization. Nine of these IRSRs are relevant to postclosure performance assessment and provide regulatory guidance in the form of:

- Descriptions of the key technical issues and associated subissues considered important to the evaluation of repository performance
- Explanations of NRC technical review methods and acceptance criteria expected to be used in reviewing performance assessment aspects of the DOE program (e.g., VA (DOE 1998a) and SR)
- Status of key technical issue subissue resolution achieved at the NRC staff level.

The IRSRs relevant to postclosure performance assessment address the following nine topical areas:

1. Total System Performance Assessment and Integration
2. Container lifetime and source term
3. Evolution of the near-field
4. Radionuclide transport
5. Unsaturated and saturated flow under isothermal conditions
6. Thermal effects on flow
7. Repository design and thermal mechanical (TM) effects
8. Structural deformation and seismicity
9. Igneous activity.

These topical areas also correspond to the core key technical issues that have been used to structure the NRC high-level waste program (Center for Nuclear Waste Regulatory Analysis, SRI 1997, pp. 1 through 4).

The NRC staff has recently indicated (NRC 1998a, p. 8) that the technical review methods and acceptance criteria contained in the IRSRs will be consolidated into those criteria contained in the TSPA&I. The TSPA&I has been given greater importance by the NRC and will be used as the foundation for developing the NRC Yucca Mountain Review Plan for a potential LA for the Yucca Mountain repository.

In this section a brief explanation of the TSPA&I subissues is provided, along with summaries of the specific DOE program activities currently underway to address them.

2.3.1 U.S. Nuclear Regulatory Commission Total System Performance Assessment and Integration Issue Resolution Status Report Subissues

Relative to the objectives of this report, the NRC TSPA&I (NRC 1998a) is of central importance to preparation of the safety case for the Yucca Mountain repository. The TSPA&I identifies the following five subissues:

1. Demonstration of overall performance objective
2. Demonstration of multiple barriers
3. Model abstraction
4. Scenario analysis
5. Transparency and traceability of the analysis.

Summary descriptions for each of these subissues are presented in the text that follows.

Subissue 1–Demonstration of overall performance objective focuses on the approach to be used by DOE to demonstrate compliance with the individual dose or risk standard. This regulatory standard will be set by the EPA and subsequently adopted in the final implementing rule, at proposed 10 CFR 63 (64 FR 8640). A critical aspect of the DOE compliance demonstration will be to show that the performance objective is met with reasonable assurance (NRC 1998a, p. 3).

Subissue 2–Demonstration of multiple barriers is concerned with the DOE performance assessment demonstrations that the repository subsystems and components are effective and diverse, and ensure resiliency of the repository system. This quantitative demonstration is not to include demonstration of compliance with the numerical subsystem performance objectives of 10 CFR 60, because they are not required in the proposed NRC implementing rule.

Subissue 3–Model abstraction, or simplification of detailed processes, focuses on requirements for defensible model abstractions and their integration into the overall TSPA model. Specifically, this subissue requires documentation of information (e.g., field and laboratory data used in developing the conceptual framework, or process level model used as a basis for the model abstractions), verification of the consistency of the abstractions, and explanation of their integration (e.g., couplings, dependencies) into the overall system model.

Subissue 4–Scenario analysis addresses the attributes of an acceptable DOE methodology for identifying, screening, and selecting the FEPs to be included in the TSPA. The FEPs that could potentially affect future repository performance are used in formulating scenarios. Guidance is provided on the construction of scenario classes, assignment of probabilities to scenario classes, and their incorporation into an overall system performance. As noted in Section 2.2, the proposed NRC rule provides criteria for use in screening FEPs and scenarios.

Subissue 5–Transparency and traceability of the analysis describes the NRC expectations for clarity and completeness of the information potentially presented by DOE in the TSPA-SR. Specifically, the technical basis for the TSPA must be sufficiently transparent and traceable to facilitate an independent analysis by the NRC staff.

2.3.2 U.S. Department of Energy Program Activities Addressing Total System Performance Assessment and Integration Issue Resolution Status Report Subissues

Because the TSPA&I, Revision 1, is only partially complete, some of the subissues cannot be addressed fully at this time. The NRC is in the process of developing the review methods and acceptance criteria for Subissues 1, 2, and 5. As noted in the TSPA&I (NRC 1998a, p. 4), the NRC intends to provide the review methods and criteria for these three subissues in Revision 2 of the IRSR. The remaining two subissues, however, can be addressed in more detail in this section.

2.3.2.1 Addressing the Demonstration of Overall Performance Objective Subissue

The current TSPA&I, Revision 1 (NRC 1998a), does not presently contain technical review methods and acceptance criteria for Subissue 1, Demonstration of Overall Performance Objective. However, specific regulatory guidance for this subissue is expected to be in the next revision of the TSPA&I IRSR (NRC 1998a, p. 7). The proposed NRC rule, under proposed 10 CFR 63.114 (64 FR 8640), outlines the requirements for a TSPA conducted for an LA. Characteristics of the reference biosphere and critical group, under proposed 10 CFR 63.115 (64 FR 8640), provide additional requirements for that part of the TSPA whereby the doses are calculated.

It is anticipated that the information needed by the NRC staff to independently check the DOE TSPA calculations will largely be documented in the TSPA-SR. Additional information useful to the NRC staff is expected to be in the set of PMRs (and associated AMRs written in accordance with QA procedure AP-3.10Q, *Analyses and Models)*.

2.3.2.2 Addressing the Demonstration of Multiple Barriers Subissue

As in Subissue 1, the IRSR does not presently contain review methods and acceptance criteria for Subissue 2, Demonstration of Multiple Barriers. The IRSR, however, indicates (NRC 1998a, p. 7) that specific guidance for this subissue will be in Revision 2. The NRC rule for disposal of high-level waste in a geologic repository at Yucca Mountain, under proposed 10 CFR 63.114(j) (64 FR 8640), contains limited guidance on requirements for describing the performance capability of multiple barriers in terms of intermediate outputs. For the case of the DOE TSPA approach, the following would be examples of intermediate outputs: waste package lifetimes, fraction of waste packages contacted by seeping water, flow rate of seeping water, and waste package radionuclide release rates.

The TSPA-SR is expected to contain detailed information on identification of barriers, quantitative description of barrier capabilities, and identification of processes affecting the performance of the natural barriers. Additional information pertinent to this subissue may also be contained in the set of PMRs (and associated AMRs).

2.3.2.3 Addressing the Model Abstraction Subissue

For this subissue, the IRSR presents generic technical acceptance criteria considered by the NRC to be essential to a defensible assessment methodology for the repository system. These criteria address five aspects of the model abstraction subissue:

- Data and model justification (focusing on sufficiency of data to support the conceptual basis of the model abstraction)
- Data uncertainty and verification (focusing on the technical basis for bounding assumptions and statistical representations of uncertainties and parameter variabilities)
- Model uncertainty (focusing on alternative conceptual models consistent with available site data)
- Model verification (focusing on testing of model abstractions using detailed process level models and empirical observations)
- Integration (focusing on appropriate and consistent coupling of model abstractions).

These five criteria have been applied and customized by the NRC staff to each of the 14 KESAs that are illustrated in Figure 2.3-1.

As stated in the IRSR, the NRC staff will review the DOE TSPAs at the level of individual KESAs to determine the acceptability of the DOE model abstractions for use in a LA. Although the DOE system model is not organized using the KESAs, the TSPA components (which are described in Section 3) can be correlated to the KESAs.

The first four acceptance criteria are expected to be addressed by the various PMR reports, which will present the relationships between field and laboratory data, process level models, and model abstractions. The fifth acceptance criteria on integration will be addressed in the TSPA-SR.

2.3.2.4 Addressing the Scenario Analysis Subissue

The IRSR presents review methods and acceptance criteria that require the DOE TSPA methodology to incorporate the following five components or steps in the scenario analysis:

1. Identification of an initial list of FEPs
2. Classification of the FEPs
3. Screening of the list of FEPs
4. Formation of scenario classes from the reduced list of FEPs
5. Screening the scenario classes.

Originally developed by the NRC (Cranwell et al. 1990), this scenario analysis procedure was first implemented by the NRC staff in their iterative performance assessment Phase 2 analysis (NRC 1995a) of the proposed repository at Yucca Mountain. The YMP has adopted a very similar procedure that is described in Section 2.1 and in Swift et al. (1999). In the TSPA-SR methodology, IRSR Steps 1 and 2 have been combined and a new Step 5 has been added to clarify the linkage between scenario development and the TSPA-SR analysis.

Step 1: Identification of Initial List of FEPs–To satisfy this acceptance criteria for this analysis component, an electronic database of FEPs has been developed using the draft NEA FEP database and other more site-specific FEPs identified by the YMP staff. The YMP electronic FEP database (Swift et al. 1999) currently has an initial list of more than 1,700 FEPs (see Section 2.2).

Step 2: Classification of the FEPs–The IRSR acceptance criteria for this step will be met by inclusion of the FEP classification in the electronic database. As described in Section 2.2, FEPs are classified as primary and secondary. They are also grouped following screening (Step 3) into EFEPs (i.e., having a probability of occurrence of 1) and DFEPs (i.e., having a probability of occurrence of less than 1, thus affecting overall system performance).

Step 3: Screening of FEPs–To satisfy the IRSR acceptance criteria for this step, screening of the FEPs will be performed using the regulatory screening criteria contained in the final NRC rule. Specifically, under proposed 10 CFR 63.114 (64 FR 8640), the NRC provides specific probability and consequence criteria for use in screening of FEPs. The results of this screening will be documented in the FEPs electronic database, which will contain:

- Screening arguments for inclusion or exclusion of the FEP
- References to supporting documentation on probability assignment and consequence analysis
- Statement of disposition for FEPs to be included in the TSPA.

In addition, the FEPs remaining in the reduced list would be used in constructing scenarios.

Step 4: Formation of Scenario Classes–The specific acceptance criteria for this step will be fulfilled by documenting the logic used in constructing the scenario classes (using the retained FEPs). The construction process will follow the diagrammatic approach presented in NRC (1995a, pp. 3 and 4) and Swift et al. (1999). This construction process will ensure that each set of scenario classes will be mutually exclusive and complete.

Step 5: Screening the Scenario Classes–The IRSR acceptance criteria for this final step will be fulfilled using the regulatory screening criteria of the proposed NRC rule (64 FR 8640), previously described under Step 2. The technical basis for the scenario class probabilities used in the screening will be documented, including the rationale for inclusion in and exclusion of scenario classes from the TSPA.

2.3.2.5 Addressing the Transparency and Traceability of the Analysis Subissue

The current TSPA methodology IRSR, Revision 1, does not contain technical review methods and associated acceptance criteria for Subissue 5, Transparency and Traceability. However, specific guidance is expected to be in Revision 2 of the IRSR (NRC 1998a, p. 90).

As in the case of Subissues 1 and 2, it is anticipated that the information needed by the NRC staff to independently check the TSPA calculations will largely be contained in the TSPA-SR. Additional information useful to the NRC staff may also be contained in the set of PMRs (and associated AMRs).

2.4 PERFORMANCE ASSESSMENT PEER REVIEW COMMENTS

2.4.1 Performance Assessment Peer Review Panel Convened

At the request of the DOE, the Civilian Radioactive Waste Management System Management and Operating Contractor (CRWMS M&O) convened the PAPR Panel. Over a period of two years, the PAPR and their consultants worked to produce an independent technical review of the TSPA-VA (DOE 1998a, Volume 3), during the development of the methodology and through completion of the assessment. The intent of the review was to develop an independent assessment of the TSPA methodology, while considering improvements that could be made in the TSPA for the potential SR and LA.

Interim reports from the PAPR (Whipple et al. 1997a; 1997b; 1998) were based on draft documentation of the TSPA-VA, as well as formal and informal meetings with DOE staff. The PAPR *Final Report Total System Performance Assessment Peer Review Panel* (Whipple et al. 1999) was primarily based on the final VA (DOE 1998a, Volume 3) and the *Total System Performance Assessment–Viability Assessment (TSPA-VA) Analyses Technical Basis Document* (CRWMS M&O 1998a).

2.4.2 Response to Performance Assessment Peer Review Panel Comments

The PAPR provided wide-ranging and detailed comments on all aspects of the TSPA-VA. Among the 161 comments in the final report by the PAPR (Whipple et al. 1999) are issues that go beyond the TSPA methodology and the conduct of the analyses. Some of the comments focus on the adequacy of the component models used in the TSPA-VA, as well as the need for additional data and possible strategies for dealing with incomplete information through bounding analyses and engineering design alternatives. Final resolution of issues raised by the PAPR comments will be made within the context of the overall project, not just within performance assessment. Every effort will be made to address the major issues, either by developing more detailed and convincing justification of the TSPA-VA approach, by undertaking the suggested remedy, or by developing and justifying an alternative approach. The PAPR has stated that the purpose of the TSPA-VA (evaluating the probable behavior of the repository) is different from the purpose of an LA (demonstrating compliance with regulatory limits). Responses to the comments will consider the distinct technical objectives of the SR and of a potential LA.

2.5 SOFTWARE QUALITY ASSURANCE: SOFTWARE QUALIFICATION AND CONFIGURATION MANAGEMENT

Several sophisticated computer codes will be used in the development of TSPA-SR. These codes are in various stages of QA qualification. The status and objectives for software qualification and configuration management of the codes are described in this section. Some of the software has been procured (acquired) from vendors or suppliers as commercial off-the-shelf software. Some software has been developed within the YMP using QA procedures.

In addition, some software has been transferred or acquired from other CRWMS M&O facilities such as the national laboratories and the U.S. Geological Survey. The primary software codes to be used in TSPA-SR are listed in Table 2.5-1 and described further in this section.

NOTE: Table 2.5-1 is not a complete list of all software that will be utilized in TSPA-SR.

Table 2.5-1. Important Codes Proposed for Use in TSPA-SR

Code Name	Version Number	Description	QA Status
RIP	5.19.01	Total System Performance Code	Qualified
FEHM	2.00	Heat and Mass Transfer Code	Qualified
TOUGH2	1.4	Modeling of the Transport of Water, Vapor, Air and Heat	Not Qualified
WAPDEG	3.09	Waste Package Degradation Code	Software Baseline Request Part I Has Been Submitted
NUFT	2.0h	Thermal Hydrology Code	Qualified
GENII-S	1.4.8.5	Estimates Dose to Humans in the Environment	Qualified
AREST-CT	1.2	Reactive Transport Code	Software Baseline Request Part I Has Been Submitted
EQ3/6	7.2b	Geochemical Modeling of Aqueous Systems	Qualified
MING	1.0	Models Microbial Impact in Near-Field Environment	Qualified
GRIM	1.0	Shell That Performs a Series of Aqueous Geochemistry Calculations Using the EQ3/6 Code.	Software Baseline Request Part I Has Been Submitted
ASHPLUME	1.4	Estimates Distribution of Ash and Radioactive Waste Released into the Biosphere During Extrusive Volcanic Events that Intercept the Repository.	Software Baseline Request Part I and Part II Have Been Submitted

NOTE: These software are scheduled to be qualified.

RIP–The Repository Integration Program (RIP) is acquired software developed by Golder Associates (Golder Associates Inc. 1998). RIP has been developed, tested, and maintained in accordance with *Golder Associates Quality Management Plan for Seattle Operations*, an ASME-1994 *Retention of Quality Assurance Records* compliant QA 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 Associates Inc. 1998).

RIP was validated in accordance with CRWMS M&O QA procedures QAP-SI-0, *Computer Software Qualification,* and QAP-SI-3, *Software Configuration Management.* CRWMS M&O control of RIP will include process controls for installation and preparation of a Software Qualification Report.

A new Microsoft Windows version of RIP is in development and may be completed in time for use in TSPA-SR. If the determination is made to use this new version, it will be validated using the new software qualification and configuration procedures that are in effect (i.e., AP-SI.1Q, *Software Management*).

FEHM–The finite element heat and mass transfer code was adapted for use at Yucca Mountain by Los Alamos National Laboratory. FEHM was verified through rigorous and complete testing of the model (in accordance with the requirements of QAP-SI-0) 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. Test cases and comparisons were performed to verify the capabilities of FEHM, including tests of thermodynamic functions, two-dimensional and three-dimensional (3-D) heat conduction, heat and mass transfer, and fracture transport/matrix diffusion. Additionally, FEHM results were compared to National Bureau of Standards Steam Table data and TOUGH2 results (Zyvoloski et al. 1995).

The approach used in the TSPA-SR to dynamically link FEHM to RIP requires special treatment to ensure traceability and integrity of data transfer between the two codes. RIP can call FEHM as a Dynamically Linked Library file, thus eliminating the need to modify any of the RIP or FEHM algorithms. This link and the accuracy and correctness of data being transferred and used between these two codes will be verified, validated, and tested. Simple data passing tests will be performed prior to the initiation of the TSPA-SR calculations to confirm that parameters are being correctly passed between the two codes.

FEHM is under configuration management control for use in TSPA-SR.

TOUGH2–The TOUGH2 code (Pruess 1991) was developed by Lawrence Berkeley National Laboratory. For software qualification purposes, TOUGH2 is officially considered to be developed software. TOUGH2 is a multidimensional numerical code used for simulating the transport of water, vapor, air, and heat in porous media. TOUGH2 (V1.4) is being verified and validated by Lawrence Berkeley National Laboratory in accordance with AP-SI.1Q.

WAPDEG–The WAPDEG code is software developed for the YMP by the CRWMS M&O QA Performance Assessment Organization. The WAPDEG code is used to simulate waste package degradation and will be further developed and tested in accordance with CRWMS M&O QA procedure AP-SI.1Q. Configuration management of the software will be controlled by CRWMS M&O AP-SI.1Q. The code is expected to be verified and validated for TSPA-SR.

NUFT–Nonisothermal Unsaturated-Saturated Flow and Transport model is a suite of multiphase, multicomponent models for numerical solution of nonisothermal flow and transport in porous media (Nitao 1998). 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 (unqualified) code for a wide range of problems related to decay-heat-altered nonisothermal flow and transport at Yucca Mountain (Wilder 1996).

GENII-S–GENII-S, a system of seven computer codes, is 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 (ICRP). The codes were originally developed in accordance with the Pacific Northwest National Laboratory QA program (Leigh et al. 1993).

AREST-CT–The analyzer of radionuclide source-term with chemical transport 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 currently is being modified and updated by the CRWMS M&O PAO in accordance with AP-SI.1Q.

EQ3/6–EQ3/6 is a computer program for reaction-path modeling of geochemical systems developed by Lawrence Livermore National Laboratory (LLNL) (Wolery 1992a; 1992b; Wolery and Daveler 1992).

MING–The microbial impacts to the near-field environment geochemistry code has been developed by the CRWMS M&O (1998d). The MING code will be used to estimate the impacts of microbes on 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 temperature and 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 nutrient cycle of the microbes are introduced into the groundwater passing through the repository.

GRIM–The geochemical repository integration model is a software shell that allows the user to perform a series of aqueous geochemistry calculations using the EQ3/6 code. GRIM was originally designed so researchers could simulate geochemical interactions in radioactive waste facilities (the software may also be used to simulate geochemical interactions in other complex systems). The code is being developed in accordance with AP-SI.1Q. Performance assessment may use the code linked with the EQ3/6 geochemical process model to simulate the time evolution of the geochemical environment in and around the waste disposal area at the Yucca Mountain nuclear waste facility. This link and the accuracy and correctness of data being transferred and used between these two codes will be verified, validated, and tested.

ASHPLUME–The ASHPLUME code will be used to evaluate the consequences of extrusive volcanic events by estimating the distribution of ash and radioactive waste released into the biosphere during volcanic events that intercept the repository. The code implements a version of the mathematical model for ash dispersion given by Suzuki (1983).

ASHPLUME Version 1.0 (Jarzemba et al. 1997) was developed by the Southwest Research Institute Center for Nuclear Waste Regulatory Analyses for use in NRC performance assessments. The CRWMS M&O plans to acquire Version 1.0 and modify it for use in the TSPA-SR. The modified code will be designated Version 1.4. The CRWMS M&O plans to qualify ASHPLUME Version 1.4 in accordance with the requirements of AP-SI.1Q.

2.5.1 Configuration Management

All of the codes that are used to support TSPA-SR will be placed under the controls of the CRWMS M&O YMP configuration management program. The software configuration management program is documented in CRWMS M&O procedure AP-SI.1Q. The software configuration management program includes software configuration identification, configuration control, and configuration status accounting.

2.5.1.1 Configuration Identification

Software configuration identification, including version or revision, is provided through the use of a unique software tracking number that is assigned to each individual software product. A series of document identifiers and media identifiers relate these baseline elements to the associated software tracking number and enables cross-referencing of the individual baseline elements.

2.5.1.2 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 or defect reports from the Responsible Manager.

2.5.1.3 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.

2.6 APPROACH TO TRANSPARENCY AND TRACEABILITY

A significant part of the TSPA-SR is communicating the analyses and results in a clear, efficient manner so the work can be properly evaluated by all stakeholders. Two key aspects of this communication are transparency and traceability.

Transparency includes imparting a high level of understanding to the stakeholders, many of whom are not technically sophisticated in the nuances involved in radioactive waste disposal. The use of graphics and multiple levels of detail in the documentation is of crucial importance to transparency.

Traceability includes developing the documentation of all analysis decisions, models and data so that the results are reproducible by other analysts without intervention from the project analysts. Configuration control of software (described in Section 2.5) and data are imperative to traceability.

The technical complexity of TSPA-SR requires evaluation of uncertainties in the processes and the rates of these processes that will occur in the disposal system in the future. Forecasting the performance of the system with models attempts to establish the limits of the possible performance outcomes of the disposal system. The forecasting is limited by available data and our current ability to assess what might happen to the disposal system through the course of time. Processes that are linked to, or provide feedback to, other processes compound the uncertainty in the behavior of the system through time. Describing the uncertainties in the system presents a significant challenge to providing transparency.

The overall approach to providing a transparent and traceable document for the TSPA-SR involves developing a clear analysis method, followed by development of the text and graphics necessary to meet the objectives. The analysis method is presented in this document. The documentation will require coordination of technical integrators, technical specialists, graphic specialists, technical editors, and production specialists to provide the transparency and traceability that is desired.

Developing understanding of the method and results of the TSPA requires a multilevel demonstration of the analyses. Graphics and text will be developed to provide information appropriate to a specific audience. Several levels of detail will be used in communicating results, depending on the audience. A progression of documents from complex to simple is envisioned to satisfy the mix of audiences comprising the various stakeholders and reviewers of the TSPA-SR.

Transparency hinges on an easy-to-understand graphical portrayal of the physical processes evaluated by the models. In particular, the figures showing model conceptualization must be at the appropriate level of detail for the technically literate, but not radioactive waste literate, person to quickly understand. Graphical specialists will work with the performance assessment analysts to update these figures from those used in the TSPA-VA. The progression and improvement in these conceptual figures from previous performance assessments is notable.

As described in Section 3, the analyses will be discretized into several parts, for ease of computation and clarity of presentation. Each part has key processes associated with it. These processes will be captured graphically. The individual discrete analyses are linked together to develop the TSPA. The portrayal of this linkage and the inherent assumptions is important to the overall transparency of the analyses.

The text of the TSPA-SR will be initially developed by the performance assessment analysts, reviewed by a technical editor and then sent to production. It is assumed that the analyst would need help in order to write the type of summary document required for TSPA-SR. The review by a technical editor will be oriented toward avoidance of acronyms and technical radioactive waste jargon, and providing a fresh look at the text from someone who was somewhat removed from the analysis. Consensus between the analysts and editors will be achieved in order to maintain ownership of the analyses by the authors.

It is also expected that multiple levels of review will be conducted to ensure that the documentation meets its goals for transparency and traceability. The documents will undergo extensive internal review during their development. Project reviewers will provide both technical and appropriateness reviews. In addition, external reviews of the approach and procedures may be solicited. Additional briefings and comments will be expected from the U.S. Nuclear Waste Technical Review Board (NWTRB), and the regulator, the NRC.

The traceability of the analyses requires the ability to explicitly identify the sources of data used, the version of software used, and the models used. The regulator and other interested parties need to be able to reproduce the results of the analyses without assistance from the performance assessment analysts. Explicit documentation of all steps taken in the analyses, of the software, and of the input used to generate the analyses will be available to attain the goal of traceability.

Portions of the analyses are more easily traced than others. For example, the top level of the performance assessment model hierarchy is fairly selfcontained in the TSPA code and its associated linked files, making reproducibility of that part of the analyses straightforward. However, moving down the model hierarchy and "pulling the data string" to the basis of the process models feeding performance assessment or to the data supporting the process models is more complex, but has been proceduralized for the TSPA-SR.

3. COMPONENTS OF THE TOTAL SYSTEM PERFORMANCE ASSESSMENT MODEL

Because of the difficulty in handling the complexity of the repository system in an analysis, the Yucca Mountain total system model is divided into individual parts to make the TSPA-SR analyses manageable. These parts are delineated and defined by both physical chemical processes and by the spatial location in the repository where the processes occur. Collectively, these individual parts of the TSPA analysis are called component models or process models. The methods and assumptions used for each TSPA-SR component model are described in this chapter. A large portion of the DOE site characterization program has been aimed at developing the scientific bases for the most reasonable representation of these models for the YMP and its associated engineered barriers. This scientific basis serves as the foundation for the process models used in the TSPA-SR.

Although all of the processes will be strongly interrelated in the actual repository system, the assumption is made that the components can be treated separately if a consistent set of boundary conditions and scenarios are rigorously maintained among all the related components. This chapter (Sections 3.1 through 3.9) addresses the conceptualization of nine component models (eight for the nominal scenario, plus one for the disruptive scenario that utilizes all of the other eight) and the implementation of these components into the performance assessment analyses. This chapter also describes how these components are recombined into the total system model and a listing of the input data vectors required for each model (Section 3.10). The component models and their corresponding key attributes and factors of the repository safety strategy (introduced in Chapter 1) are listed in Table 3-1.

To ensure that the TSPA-SR would be based on the most current scientific knowledge, a series of workshops were held in 1998 and 1999 to bring together YMP scientists, engineers, and performance assessment analysts. These individuals consisted of DOE, national laboratory, U.S. Geological Survey, and CRWMS M&O contractor scientists and engineers. Observers at these workshops included technical staffs from regulatory agencies (e.g., the NRC and EPA) and their contractors, and individuals from external oversight groups such as the NWTRB. The aim of these workshops was twofold: (1) to develop a strategy for identifying and incorporating the key aspects of the individual process models into the TSPA-SR analyses, and (2) to ensure that engineering and scientific work across the YMP was integrated and focused on those safety factors most important to performance. Each workshop culminated in a plan or plans for incorporating that component in the TSPA-SR and linking that component to other portions of the TSPA. These workshops are listed in Table 3-1, along with the associated TSPA component model and the section in this chapter where the component model is described.

Table 3-1. Factors Affecting Expected Postclosure Performance and Their Corresponding TSPA-SR Component Model and Associated TSPA Workshop

Key Attributes of System	Factors	TSPA Component	TSPA-SR Workshop	Section
Water Contacting Waste Package	Climate	UZ Flow and Transport	UZ Flow and Transport 12/14-15/98, Albuquerque, NM	3.1
	Infiltration			
	UZ Flow Above Repository			
	Seepage into Drifts	Thermal Hydrology and UZ Flow and Transport	Thermal Hydrology and Coupled Processes Workshop 3/24-25/99, Albuquerque, NM and UZ Flow and Transport 12/14-15/98, Albuquerque, NM	3.1 and 3.2
	Coupled Processes - Effects on UZ Flow			
	Coupled Processes - Effects on Seepage			
	Environment on Drip Shields	IDGE	IDGE and EBS Transport 4/13-15/99, Las Vegas, NV	3.3 and 3.6
		EBS Transport		
	Performance of Drip Shields	Waste Package	Waste Package and Drip Shield Degradation 4/20-21/99, Las Vegas, NV	3.4
Waste Package Lifetime	Environment on Waste Package	Thermal Hydrology	Thermal Hydrology and Coupled Processes 3/24-25/99, Albuquerque, NM	3.2 and 3.3
		IDGE	IDGE and EBS Transport 4/13-15/99, Las Vegas, NV	3.3 and 3.6
		EBS Transport		
	Performance of Waste Package Barrier	Waste Package	Waste Package and Drip Shield Degradation 4/20-21/99, Las Vegas, NV	3.4
Radionuclide Mobilization and Release from the EBS	Environment Within Waste Package	Waste Form	Waste Form Workshop 2/2-4/99, Albuquerque, NM	3.5
	CSNF Waste Form Performance			
	DSNF, Navy Fuel, Plutonium Disposition Waste Form Performance			
	HLW Glass Waste Form Performance			
	Solubility Limits of Dissolved Radionuclides			
	Colloid Associated Radionuclide Concentrations			
	In-Package Radionuclide Transport			
	Transport Through Invert	EBS Transport	IDGE and EBS Transport 4/13-15/99, Las Vegas, NV	3.6

Table 3-1. Factors Affecting Expected Postclosure Performance and Their Corresponding TSPA-SR Component Model and Associated TSPA Workshop (Continued)

Key Attributes of System	Factors	TSPA Component	TSPA-SR Workshop	Section
Transport Away from the EBS	Advective Pathways in the UZ	UZ Flow and Transport	UZ Flow and Transport 12/14-15/98, Albuquerque, NM	3.1
	Retardation of Radionuclide Migration in the UZ			
	Colloid Facilitated Transport in the UZ			
	Coupled Processes - Effects on UZ Transport			
	Advective Pathways in the SZ	SZ Flow and Transport	SZ Flow and Transport and Biosphere 2/17-19/99, Albuquerque, NM	3.7
	Retardation of Radionuclide Migration in the SZ			
	Colloid Facilitated Transport in the SZ			
	Dilution of Radionuclide Concentrations in the UZ and SZ	Biosphere		3.8
	Biosphere Transport and Uptake			
Effects of Disruptive Events	Factors for Igneous Activity Scenarios	Disruptive Events	Disruptive Events 2/9-11/99, Albuquerque, NM	3.9
	Factors for Seismic Activity Scenarios			

The major component models, and some of their associated submodels, are illustrated in the context of the geologic setting and engineered barriers of the potential Yucca Mountain repository (Figure 3-1). Submodels represent a further division of the major component models. These submodels can exist at various levels of complexity and computational detail. For example, three submodels of the UZ flow and transport component model include a conceptual climate model based on interpretation of past climates, a numerical infiltration model that explicitly simulates relevant processes at Yucca Mountain, and an ambient (i.e., not thermally perturbed) seepage model that uses detailed numerical calculations to support parameter distributions used in a simplified TSPA abstraction.

The model components and factors related to limiting the amount of water contacting the waste package, the first key attribute in the repository safety strategy, include climate, infiltration, UZ flow, mountain-scale and drift-scale coupled processes (including thermal hydrology), seepage (into the drift and through degraded drip shields), IDGE, and degradation of the drip shield. Together, these components define the temporal and spatial distribution of water flow through the unsaturated tuffs above the repository at Yucca Mountain and the temporal and spatial distribution of water seeps onto the waste packages. There could be short- or long-term (thousands to tens of thousands of years) climate variations. In addition, the thermal regime generated by the decay of the radioactive wastes can mobilize connate water over the first hundreds to thousands of years. For these reasons, the amount of water flowing in the rock and seeping onto the waste packages is expected to vary with time.

The model components related to long waste package lifetime, the second key attribute of the repository safety strategy, include all the above components plus waste package degradation. Together, these components define the spatial and temporal distribution of the times when waste packages are expected to breach. These thermal, hydrologic, mechanical, and geochemical processes acting on the surface of the waste packages are the most important environmental factors affecting the waste package corrosion rate.

The model components related to slow mobilization and release of radionuclides from the EBS, the third key attribute, include all the above components plus coupled processes within the package (including seepage through the package), waste form degradation (including cladding degradation for CSNF), radionuclide mobilization (including dissolved concentration limits and colloid associated concentrations), and radionuclide transport through the EBS. Together, these components lead to a determination of the spatial and temporal distribution of the mass of radioactive wastes released from the waste packages.

The model components related to transport away from the EBS (i.e., through the natural barriers and biosphere), the fourth key attribute of the repository safety strategy, include all the above components plus radionuclide transport through the UZ and SZ, dilution from pumping, and radionuclide transport in the biosphere. Together, these components determine the spatial and temporal variation of radionuclide concentrations in groundwater. The groundwater concentration ultimately yields the mass of radionuclides that may be ingested or inhaled by individuals exposed to that groundwater, which in turn causes a level of radiological dose or risk associated with that potential exposure. Radionuclide transport may occur by advection (radionuclide movement which occurs with the bulk movement of the groundwater) or diffusion (radionuclide movement which occurs because of a concentration gradient). The concentration depends on the mass release rate of the radionuclides and the volumetric flow of water along the different pathways in the different components. If the volumetric flow of water from the pumping centers is greater than the volumetric flow in which the radionuclides are contained, then dilution of radionuclide concentrations can occur at the pumping well.

Each of the above key attributes and TSPA model components are used to describe the nominal behavior of the Yucca Mountain repository system. In addition, other FEPs can occur that could alter the behavior of the system. However, these FEPs have a sufficiently low probability of occurring over the period of interest that they are usually not considered in the nominal behavior. They may essentially be classified as unanticipated processes and events. Examples of such disruptive events include igneous activity, seismic activity, criticality events, and human intrusion. The potential consequences associated with unanticipated processes and events are usually considered in the TSPA analyses as separate scenarios from the nominal scenario, and then recombined based on probabilities to give a total expected dose (see Section 4.4). However, for the TSPA-SR, seismic events may be included as a part of the nominal scenario, criticality is of such low probability that it may be screened out by the FEPs screening process, and, based on proposed regulations (64 FR 8640), human intrusion will be treated as a separate performance assessment analysis (see Sections 3.9 and 4.7).

3.1 UNSATURATED-ZONE FLOW AND TRANSPORT

The UZ is that portion of the geologic medium where rock voids, pores, and fractures are partially filled with water. The UZ at Yucca Mountain spans the volcanic rocks, from the ground surface to the water table. The UZ is distinct from the region below the water table, referred to as the SZ, where all pores in the rocks are completely filled with water. However, within the UZ there are some locally saturated regions called perched water zones.

The UZ is a component of the natural barrier system. It contributes to repository performance by:

- Reducing the amount of water reaching waste by combined surficial (e.g., precipitation lost to runoff and evapotranspiration) and subsurface (e.g., diversion of flow around emplacement drifts) processes
- Providing the hydrochemical environment in which the EBS functions
- Delaying the transport of aqueous and colloidal radionuclides to the SZ
- Serving as a buffer against the impact of climate changes on UZ flow.

3.1.1 Introduction

The current Yucca Mountain climate is classified as semiarid. On the average, the site receives approximately 170 mm/year of precipitation. Of that amount, about 95 percent is lost by runoff and evapotranspiration. The remaining five percent infiltrates into the volcanic rocks, which consist of alternating layers of ash flow and air fall tuffs. Because of variations in soil cover thickness and topography, and spatial variability of precipitation, infiltration at the site is spatially variable. Observations at surface locations with significant soil cover indicate that meteoric water does not reach the underlying bedrock, but instead is returned to the atmosphere by evapotranspiration. In contrast, more net infiltration of meteoric water occurs alongside slopes and ridgetops, where the soil cover is thin, or fractured rock is exposed. In addition, channels, which occupy a small portion of the site, have the potential to make significant contributions to local net infiltration during runoff events.

Stratigraphic information shows that the tuff layers dip to the east at about 5 to 10 degrees and are offset by a series of north-striking, west-dipping normal faults. The main repository block is bordered on the west by the Solitario Canyon fault and on the east by the Bow Ridge fault. The Ghost Dance fault extends in a north-south direction within the block (the repository design for SR has all waste emplaced to the west of the Ghost Dance fault). A more poorly delineated, northwest-trending fault, the Drill Hole Wash structure, extends along the northern boundary of the proposed repository.

The UZ at Yucca Mountain is about 750-m thick and is composed of a number of major hydrogeologic units. These units include the Tiva Canyon welded (uppermost), Paintbrush nonwelded, Topopah Spring welded, Calico Hills nonwelded, and Crater Flat undifferentiated. The welded units typically have low matrix porosities and high fracture densities, whereas the nonwelded tuffs have relatively higher matrix porosities and lower fracture densities.

The Paintbrush nonwelded unit appears to play an important role in the UZ, slowing and distributing the vertical flow of percolating water. In contrast, water flow through the Topopah Spring welded unit is believed to be highly heterogeneous, ranging from low conductance zones (associated with widely dispersed or poorly connected fracture systems) to very transmissive features. Below the repository, parts of the Calico Hills nonwelded unit were altered to zeolitic form during the cooling period after initial formation. The zeolitized layers can have very low permeability; water has been found to be perched on the Calico Hills nonwelded zeolitic unit in several drill holes, indicating that water cannot drain freely in those locations. The zeolite minerals in the Calico Hills unit have significant potential to adsorb certain dissolved radionuclides. There is, however, uncertainty regarding whether the radionuclides transport through the zeolites, where they can be adsorbed, or are carried around the zeolites by water draining laterally over the top of the zeolitic layers because of their low permeability.

3.1.2 General Description of Process Models and Abstractions

The UZ component of the TSPA includes five major aspects of flow and transport in the UZ: climate, infiltration, mountain-scale water flow, seepage into emplacement drifts, and radionuclide transport. The climate subcomponent provides future histories of precipitation and air temperature, which serve as inputs to the infiltration subcomponent; of water table elevation, which is used as a bottom boundary condition for the mountain-scale-flow subcomponent and the thermal-hydrology TSPA component; and of changes in SZ flux, which are used by the SZ flow and transport TSPA component. The infiltration subcomponent provides net infiltration of meteoric water at the surface, which is used as a top boundary condition for the mountain-scale-flow subcomponent and the thermal-hydrology TSPA component. The mountain-scale-flow subcomponent provides water velocity and saturation, which define the flow field for the radionuclide-transport subcomponent. The seepage subcomponent provides seepage flux into the drifts, which is used by the IDGE and EBS flow and transport TSPA components. The radionuclide-transport subcomponent provides the mass flux of radionuclides at the water table over time, which is used as input to the SZ flow and transport TSPA component.

3.1.2.1 Climate

There is not a climate process model for Yucca Mountain; the climate abstraction is based on paleoclimate studies. Paleoclimate data are used to estimate precipitation and temperature at Yucca Mountain during periods in the past. The past climates are extrapolated to the future by means of the Milankovitch cycles, which are cycles in the earth's orbital and rotational parameters that have been observed to correlate to the earth's climate cycles. Both global and local paleoclimate data are used. Global data (e.g., seabed sediments) have been used to show the correlation of climate variations with the Milankovitch cycles, and data from the Yucca Mountain area (e.g., packrat middens) are used for information on the impact of climate changes at Yucca Mountain. Climate information is passed to the infiltration model in terms of climate analogs, which are present-day locations that have climate conditions (and, in particular, mean annual precipitation and mean annual temperature) similar to those inferred for Yucca Mountain at some time in the past or future.

In addition, paleohydrologic data (e.g., paleospring deposits) are used to estimate how the water table fluctuates with climate. Water table changes, plus calculated infiltration changes, are used to estimate changes in SZ groundwater flux for future climates.

3.1.2.2 Infiltration

Infiltration maps for present-day and future climates will be generated using the INFIL computer code (the version used will be baselined appropriately). The infiltration model covers an area of approximately 10 km × 20 km, with cells that are 30 m × 30 m. Important processes in the model include:

- Precipitation
- Surface water runoff and run-on
- Evapotranspiration
- Changes in soil and shallow bedrock moisture.

The surface water (runoff and run-on) model has been improved since the TSPA-VA (the model and assumptions used for TSPA-VA are described in CRWMS M&O 1998a, Chapter 2, Section 2.4.2). In addition, processes have been added to the model to better represent infiltration under future climates, including:

- Temperature dependence, to take into account changes in temperature under different climates

- Vegetation dependence, to take into account changes in types of vegetation under different climates

- Accumulation and melting of snowpack under colder climates.

The precipitation and temperature inputs for the model are generated with a stochastic model that uses actual precipitation and temperature records from the appropriate analog site as input. This approach is necessary because many weather records, including those from the Yucca Mountain area, are less than 50 years old. A 100-year record is desired for input to the infiltration model so that the results are not overly dominated by short-term fluctuations. (Analog sites are needed even for present conditions, because records at Yucca Mountain itself do not go back far enough in time.)

The only abstraction needed for the infiltration model is spatial and temporal averaging. The mesh for the flow models is coarser than the infiltration model mesh, so infiltration for a flow boundary cell is typically obtained by averaging over multiple infiltration cells.

3.1.2.3 Mountain-Scale Unsaturated-Zone Flow

A full 3-D mountain-scale model is being developed to simulate the UZ flow field, using the TOUGH2 computer code (the version used will be baselined appropriately). The model domain is approximately 5 km × 9 km × 800 m. The cell size is variable, with smaller cells along faults and within the repository area. The model grid explicitly incorporates a number of major faults, including Solitario Canyon, Ghost Dance, and others. For SR, the model grid within the repository is being modified so that it better matches the planned repository, which will be useful for estimating conditions in particular drifts, if desired.

Flow is modeled using a dual-permeability formulation, which means that water flow is taken to be through fracture and matrix continua, with flow interactions between the two continua. A new active-fracture model for fracture-matrix interactions (Liu et al. 1998) is being used in the model, providing a better theoretical basis for interactions than the one used for the TSPA-VA (CRWMS M&O 1998a, Chapter 2, Section 2.4.3.3). The active-fracture model is based on the fact that only a portion of the connected fractures may be active in conducting liquid water. The model describes gravity-dominated, nonequilibrium, preferential liquid water flow through fractures, including a reduction factor for the interface area between fractures and matrix. The area-reduction factor depends on the relative number of active fractures in a connected fracture network and is a function of liquid saturation and water flux in the fracture continuum.

Calibration of the mountain-scale flow model is being performed using the ITOUGH2 computer code (the version used will be baselined appropriately), which uses an inverse method to determine the best fit to observed data by adjusting input parameter values within specified ranges. Data used in model calibration include moisture saturation, water potential, pneumatic pressure, and perched water levels. Isotope, geochemical, and temperature data are also used to constrain the flow solution.

An alternative conceptual model of flow and transport around or through the perched water is being investigated. In the VA, the perched water locations acted as barriers to flow (DOE 1998a, Sections 3.1.3.2 and 3.6.3.1). Thus, flow was diverted laterally above the perched water. An alternative conceptualization is that flow is primarily vertical, through the perched water. The flow-around model is expected to be more conservative, because the lateral flow and subsequent draining to the water table is rather rapid in the model. However, if flow is through the perched water there could be a significant residence time in the perched water and there might be increased contact of radionuclides with the highly sorbing zeolites in the Calico Hills zeolitic layer. Thus, repository performance could be significantly enhanced in this alternative model.

The UZ flow fields obtained from the mountain-scale flow model are used directly, without additional abstraction, as input to the UZ transport model, requiring only a postprocessor to put them in the appropriate format for the transport code. An investigation of thermal effects on UZ flow and transport is planned, and an abstraction of these effects might be added if they are determined to be important.

3.1.2.4 Seepage Into Drifts

A drift-scale flow model is being developed for the purpose of providing estimates of seepage into emplacement drifts; that is, estimates of the amount and distribution of liquid water entering emplacement drifts. New data from seepage tests in the Exploratory Studies Facility (ESF) are expected to provide a better basis for the conceptual model and parameter ranges. The model domain is represented as a heterogeneous medium with the rock properties (primarily fracture permeability, but possibly other properties as well) varying spatially. The TOUGH2 computer code (the version used will be baselined appropriately) is used with a fine grid (grid spacing of

0.5 m or less). The flow conceptual model will either be dual permeability, consistent with the mountain-scale flow model, or a simplified fracture only model, as was done for the VA (DOE 1998a, p. 3-12). A fracture-only model is conservative compared to a dual permeability model, and computations run much faster. If matrix hydrologic properties are used, they will be consistent with the matrix properties in the mountain-scale UZ flow model, but fracture properties are not necessarily the same because of scaling issues. The mountain-scale property sets make use of pneumatic data (barometric pressure fluctuations) for fracture permeabilities. These represent very large-scale effects. The drift-scale property sets make use of smaller-scale air permeability data for fracture permeabilities.

The drift-scale flow model results will be abstracted before passing them on to other TSPA components. The abstraction is expected to be done in the same way as for the VA which was to calculate amounts of seepage and its spatial distribution for a range of important fracture hydrologic properties, and then develop probability distributions for seepage fraction and seep flow rate as functions of percolation flux (DOE 1998a, Sections 3.1.2.4 and 3.1.3.3). Seepage fraction is the fraction of waste packages or drip shields contacted by dripping water, and seep flow rate is the average flow rate of water onto those waste packages or drip shields that have dripping.

In addition, studies are planned or underway to evaluate effects of various coupled processes on seepage into drifts:

- Degradation of drifts due to mechanical and seismic stresses
- Thermal hydrologic (TH) processes
- Thermal-hydrologic-chemical (THC) processes
- Thermal-hydrologic-mechanical (THM) processes.

If these processes are found to be important, it will be necessary to abstract or bound them for the TSPA calculations.

3.1.2.5 Unsaturated Zone Radionuclide Transport

Consistent with the mountain-scale flow model, the UZ transport model will use a dual continuum conceptual model in which fracture and matrix transport are coupled through advective and diffusive transport mechanisms. Transport from the repository to the water table will be calculated in 3-D using the FEHM computer code(the version used will be baselined appropriately). The FEHM particle tracking algorithm simulates aqueous-phase and colloid-facilitated radionuclide transport processes through the UZ, including:

- Advective transport (within and between fracture and matrix continua)
- Hydrodynamic dispersion
- Matrix diffusion
- Linear sorption
- Radionuclide decay.

A colloid transport process model is being developed in conjunction with modeling being conducted for the Nevada Test Site (NTS). Observations of colloid transport at the NTS, associated with the Benham nuclear test site (Thompson 1998, pp. 11–19), provide data that can be used to calibrate the colloid model and help to build confidence in the model.

As with the UZ flow model, the UZ transport model will be used directly in the TSPA, without additional abstraction. FEHM will be coupled directly to the RIP TSPA code in the form of a dynamically linked library (the version of RIP used will be baselined appropriately). This allows considerable flexibility in the inputs and outputs, including probabilistic sampling of key uncertain input parameters. The colloid transport process model discussed above will probably be abstracted so that computation of colloid transport can be done within FEHM, although the details of the abstraction have yet to be developed.

An important improvement to the UZ transport is planned, in the form of better coupling with EBS transport at the repository and SZ transport at the water table. For the VA , releases from the EBS to the UZ were spread over rather large repository subregions (DOE 1998a, Figure 4-10). Similarly, releases from the UZ to the SZ were again spread over large repository subregions, resulting in substantial artificial dilution in some circumstances. A more detailed coupling is planned for SR, with releases spread over a more realistic area in each case.

An additional improvement is planned for the FEHM particle tracking method, with respect to the treatment of matrix diffusion. The present model for matrix diffusion is based on the assumption that the fracture spacing is large (infinite) relative to the average diffusion penetration depth from fractures into the matrix for a radionuclide being transported through the UZ. The matrix diffusion model is being revised to account for the effects of finite fracture spacing.

As for UZ flow (Section 3.1.2.3), the effects of repository heating on UZ transport will be evaluated. If these effects are found to be important, a model abstraction will be devised to incorporate them into the FEHM particle tracking method.

3.1.3 Significant Coupling with Other Models

Climate change times affect many aspects of the TSPA. The climate model (which is not a computerized numerical model, but more of a conceptual model derived from data) provides climate change times directly to the TSPA model so that it can generate the future climate history for each realization of a Monte Carlo simulation.

The climate model provides precipitation and surface temperature for future climates to the infiltration model in the form of climate analogs. Actual daily precipitation and temperature records from the analog site are used as input to a stochastic model that is used to generate simulated 100-year records.

The climate model provides water table rise for future climates to the mountain-scale UZ flow model and the thermal hydrology models. The water table location is used as a bottom boundary condition in these models.

The climate and infiltration models are used to provide changes in SZ groundwater flux for future climates to the SZ flow and transport models. These are used to scale the SZ flow fields to approximate future conditions.

The infiltration model provides net infiltration flux to the mountain-scale UZ flow model and the thermal-hydrology models. They use net infiltration as a top boundary condition.

The mountain-scale UZ flow model provides flow fields (spatial distributions of fracture and matrix saturations and percolation fluxes) to the UZ radionuclide transport model. The flow fields define the background on which radionuclide transport takes place.

The mountain-scale UZ flow model provides calibrated sets of hydrologic properties to the seepage and thermal hydrology models.

The seepage model requires percolation flux as input. Functionally, the percolation flux is input to the TSPA model, and then, during a TSPA simulation, percolation flux is passed from the TSPA model to the seepage abstraction in order to calculate the seepage quantities. In the VA, percolation flux was taken from the mountain-scale UZ flow model, averaged over the repository subregions (DOE 1998a, Figure 4-4), but for SR, percolation flux will be taken from the multiscale thermal hydrology model in order to incorporate thermal effects on seepage (more information on this is given in Section 3.2).

The seepage quantities (seepage fraction and seep flow rate) are provided to the models for in-drift geochemistry and EBS flow and transport. In the VA, seepage model results were used directly by the other engineered system models (waste package and waste form degradation) as well (DOE 1998a, Figure 3-6), but an EBS flow and transport model is being developed now (see Section 3.6). The SR design includes additional design features (drip shield and backfill) that make it more important to account for flow diversion within the emplacement drifts.

The in-drift geochemistry model requires the chemical composition of the seeping water as well as the quantity. Because temperature effects are important for chemistry, the water composition will be provided by the thermal hydrology model (see Section 3.2).

The UZ radionuclide transport model takes as its input radionuclide mass flux from the repository, provided by the EBS flow and transport model. As its output, it provides radionuclide mass flux at the water table to the SZ flow and transport model.

It is important to note that the UZ flow and transport models are not coupled to the disruptive-scenario models. Consequently, the UZ models do not include potential effects of changes in the hydrology induced by disruptive events (e.g., seismic activity, igneous activity, and faulting). The justification for excluding these disruptive events will be documented through the FEP screening process (see Section 2.2).

3.1.4 Major Assumptions

In developing the process level models for UZ flow and transport, the classical conservation laws have been used. However, a number of fundamental assumptions have been made in order to make the modeling problem tractable. The assumptions will be fully documented and justified in the UZ Flow and Transport Model PMR or its associated AMRs. Some of the important assumptions are as follows:

- Milankovitch cycles provide a basis for predicting the timing of future climate changes.

- Shallow infiltration through the soil and rock layers at the ground surface is predominantly vertical (i.e., lateral near-surface flow is negligible).

- Hydraulic behavior of the UZ is adequately described by a dual-permeability model (i.e.. fractures and matrix can be represented by interacting continua).

- Flow is quasi-steady-state (i.e., the transient periods at times of climate change can be neglected and flow can be treated as a series of steady states).

- The van Genuchten/Mualem equations adequately describe the saturation-desaturation behavior of the volcanic rocks (both matrix and fractures) under both ambient and TH conditions.

- Appropriate matrix and fracture hydraulic properties can be obtained by inverse modeling that tests the fit to matrix saturation measurements and other field data. Matrix hydraulic properties are required to be within the range of laboratory measurements. Ranges of fracture hydraulic properties are based on air permeabilities, pneumatic tests, fracture frequencies, and fracture orientations measured in drill holes and in the ESF.

- Fracture-matrix coupling is adequately represented by the active-fracture model.

- Small-scale heterogeneity does not need to be included in the mountain-scale flow model (i.e., hydrogeologic units can be treated as homogeneous).

- Discrete-fracture effects on seepage can be adequately represented by a continuum model.

- Transport in the UZ is adequately described by a dual-continuum model.

- UZ transport is dominated by advection (i.e., there is a high Peclet number), which allows use of the particle tracking model.

- Hydrodynamic dispersion is a linear function of flow magnitude and direction.

- Radionuclide sorption is reversible and described by a linear isotherm.

3.1.5 Implementation in Total System Performance Assessment–Site Recommendation

Climate change will be incorporated into TSPA-SR in the same manner as was done for the VA: by assuming a sequence of steady states, with abrupt changes from one climate state to the succeeding state (DOE 1998a, Section 3.1.2.1). The particular climate states and the climate change times will be different from those used previously, based on a detailed climate analysis that is being done. The focus is on the first 10,000 years after waste emplacement. Preliminary indications are that three climate states will be used present-day climate for approximately the first 600 years, a monsoon climate that is warmer and wetter than present for approximately the following 1,400 years, and a glacial transition climate that is cooler and wetter than present for the balance of the 10,000-year period. Treatment of longer time periods (up to one million years) for the EIS is still to be decided: one possibility would be to extend the glacial transition climate throughout the extended time period. The approach will be determined to meet the technical and consistency needs of the EIS. An uncertainty range for climate impact will be included for each future climate, with upper and lower bounds for precipitation and temperature being specified. Treatment of water table rise and changes in SZ groundwater flux will be the same as for the VA (DOE 1998a, Section 3.1.2.1), though the particular values used could possibly be different.

Infiltration will be incorporated into TSPA-SR in the same way as for the VA: by means of detailed spatial maps of net infiltration for discrete cases (DOE 1998a, Section 3.1.2.2). The uncertainty associated with the infiltration model is being developed by running it in a stochastic mode and applying probability distributions to the key uncertain input parameters. The overall uncertainty in infiltration will be a combination of the climate uncertainty discussed above and the infiltration-model uncertainty. Because of this infiltration uncertainty analysis, the weighting factors for the various infiltration cases will have a more quantitative basis.

Mountain-scale UZ flow will be incorporated into TSPA-SR in the same manner as was done for the VA: by means of detailed 3-D flow fields for discrete cases (DOE 1998a, Section 3.1.2.3). Because the variations in hydrologic parameters included in past TSPAs (e.g., variations in fracture air-entry parameter and fracture permeability in TSPA-VA) have not resulted in significant effects on overall repository performance (DOE 1998a, Section 5.1.3), current plans are to vary only infiltration. Thus, there will be three calibrated UZ flow models, for low, nominal, and high infiltration. Each of the calibrated flow models will also be run for the two future climate states. In addition, two conceptual models of flow in the perched water region will be considered, resulting in a total of 18 flow fields (three infiltration rates times, three climates times, two perched water conceptual models). If thermal effects on mountain-scale flow are determined to be important, they would probably be included by adding one or more additional time periods to the ones defined by climate, with thermally perturbed flow fields used for those periods.

The abstraction for seepage into emplacement drifts in TSPA-SR will be similar to the one for VA, with uncertainty distributions defined for seepage fraction and seep flow rate, as well as functional dependence on percolation flux (DOE 1998a, Section 3.1.2.4). An important difference is that, in order to incorporate thermal effects on seepage, time varying percolation flux obtained from the multiscale thermal hydrology model will probably be used. This would result in seepage varying throughout the thermal period rather than being quasi-steady. Time-varying seepage chemistry will also be provided (see Section 3.2). This method would imply zero seepage for a period of time when the rock around the drifts is heated above boiling. Because of concerns that such a result would be nonconservative (because it might be possible for flow in discrete channels to penetrate the boiling zone and reach the drifts), an abstraction that allows for the possibility of seepage during the boiling period is planned. One method that has been suggested is to randomly sample between zero and ambient seepage during the period when the initial model returns zero seepage.

UZ radionuclide transport will be incorporated into TSPA-SR in the same manner as was done for the VA: by coupling the transport model directly to the TSPA model (DOE 1998a, Section 3.6.2.2). As in the VA, probability distributions will be sampled for key uncertain input parameters (DOE 1998a, Section 3.6.2.3).

3.1.6 Sensitivity Cases

The TSPA-SR model, as described in the preceding section, incorporates a number of uncertain parameters that will be sampled from probability distributions during Monte Carlo simulation. Examination of the relationships between the calculated doses for individual realizations and the corresponding uncertain-parameter values will provide valuable information on the sensitivities of the model system (see Section 4.1).

In addition, a variety of one-off sensitivity analyses will be performed for the TSPA model. In these, one (or a few) parameters or submodels are varied, while all others are kept fixed at particular reference values (typically mean or median values from the probability distributions). The one-off sensitivity analyses are used to obtain additional information on which parameters and submodels have the greatest effect on repository performance. The choice of which specific parameters or submodels to vary will not be made until after the nominal case results are examined, but possible sensitivity analyses of this type include the following:

- Climate fixed at each of the three modeled climate states (that is, no climate change)
- Low, nominal, and high infiltration
- Alternative models of flow around or through the perched water
- With and without thermal effects on flow and seepage
- With and without drift degradation effects on seepage
- Seepage at 5 percent, mean, and 95 percent of the probability distribution
- Bounding seepage estimate (e.g., seepage fraction equal to 1, seep flow rate equivalent to all flow above emplacement drifts)
- Key transport properties at 5 percent, mean, and 95 percent of their probability distributions
- Matrix diffusion included and excluded.

Sensitivity analyses can also be performed at the subsystem level—that is, testing the process or abstraction models without taking the calculation all the way to dose. This type of analysis is done primarily to test the effects of key model assumptions as part of the model-development process. Possible sensitivity analyses of this type include the following:

- Flow and transport simulations with alternative assumptions about climate change timing
- Flow and transport simulations using alternative (possibly geostatistics based) conceptions of the zeolitization of the Calico Hills nonwelded unit

- Comparison of different numerical methods for the transport calculation (specifically, comparison of the particle tracking method with a standard advection-dispersion method)

- Flow and transport simulations under isothermal conditions compared to ones with repository heat included

- Seepage simulations under isothermal conditions compared with repository heat included

- Seepage simulations using alternative conceptions of drift degradation.

3.1.7 Treatment of Uncertainties

Three basic approaches are used to deal with uncertainties:

- Probability distributions for key uncertain parameters
- Alternative models for key processes
- Bounding values of parameters or bounding approximations for processes or models.

The first two methods provide quantitative estimates of the effects of the uncertainty on repository performance; the third method does not, but is sometimes used to avoid the necessity of defending uncertain assumptions. Examples of the three approaches follow.

In the TSPA-SR model, probability distributions are expected for the following parameters:

- Infiltration (discrete distribution)

- Seepage fraction and seep flow rate

- Key transport parameters, such as sorption coefficients, diffusion coefficients, fracture apertures and spacings, and colloid transport parameters.

As discussed in Section 3.1.2.3, two alternative conceptual models for flow around or through the perched water are being developed. Either the most conservative of the two will be used in the TSPA-SR, or both will be used, weighted by their relative likelihood.

As alluded to above, bounding assumptions are typically used to simplify a model and make it easier to defend. For example, using a conservative bound might reduce the amount of data needed. An example that was mentioned previously is that seepage during the thermal dry-out might be bounded (by ambient seepage or by random sampling between zero and ambient) in order to avoid having to develop a detailed model of penetration of localized flow plumes through the dry zone around the emplacement drift.

3.2 THERMAL HYDROLOGY AND COUPLED PROCESSES

3.2.1 Introduction

Models of thermal hydrology and coupled processes in the Yucca Mountain UZ are required in order to provide a reasonable assessment of the impacts of repository decay heat on the EBS and the natural geologic system in the far-field (at the scale of the mountain) and the near-field (at the scale of an emplacement drift). The in situ water and gas will change in response to the emplacement of heat-generating radioactive wastes. Repository heating will cause formation of dryout and condensate zones, and mobilization of water vapor, liquid water, and latent heat. The resulting perturbation to hydrologic processes will last for thousands of years after waste emplacement.

In addition to the hydrologic changes to the mountain, heat input also drives coupled mechanical and chemical processes. The development of thermal stresses (normal and shear) during heating will cause compressive regions around the repository, where fractures tend to close, and tensile regions, where fractures tend to open. Boiling and resultant precipitation of naturally occurring minerals may result in the reduction of fracture apertures. Regions in which condensate waters accumulate and then readily flow may result in dissolution and precipitation of minerals, potentially increasing fracture apertures in one location while reducing them in another. These processes also influence the water chemistry.

Some of the changes involving mechanical and chemical processes may be durable, affecting the flow system for tens of thousands of years, or longer, after heating subsides. It is possible that the ambient hydrologic properties of the mountain will be permanently altered as a result of repository heat. Thermal hydrology and coupled processes models provide the tools to estimate the duration and extent of thermally driven alterations to the engineered systems and the natural geologic system.

Heat will strongly influence local conditions around the waste packages and within the drifts. The thermodynamic environment in the emplacement drifts depends on the decay-heat characteristics of the individual waste packages. The thermodynamic environment is a description of physical conditions (e.g., hot, dry, humid). The drift environment affects repository performance primarily by influencing the overall lifetime of the waste packages. Heat also will alter large-scale liquid and gas flow. Heat-driven features at mountain-scale potentially include the development of large gas-phase convection cells and thermally altered liquid-phase flow fields above and below the repository.

Results of the thermal hydrology and coupled processes models will serve as inputs to both in-drift and far-field models in the TSPA-SR. The abstracted results from the THC drift-scale model and the multiscale near-field and EBS TH model provide boundary condition inputs to the EBS TSPA models used to describe the evolution of the IDGE, EBS flow and transport, waste package and drip shield degradation, and waste form degradation. An assessment of the extent and duration of the thermal perturbation on the far-field flow below the repository will be made.

Inputs to thermal hydrology and coupled processes modeling will come from a variety of sources including UZ flow and transport, repository design, EBS, and tectonics components. The hydrologic parameters and climate information are defined within the UZ flow task. Rockfall information is provided by the EBS and tectonics tasks. However, the reference design has backfill in the emplacement drifts, so rockfall information will not be required by the thermal hydrology and coupled processes component of TSPA except possibly for a no-backfill sensitivity analysis. Needed repository design specifications include mass loading, repository layout, heat output over time, and other important engineering-related inputs.

3.2.2 General Description of Process Models and Abstractions

The process models used in abstraction are the THC drift-scale model, the multiscale near-field and EBS TH model, and the THM drift-scale and mountain-scale models. The first two models provide specific results to the TSPA, as described below. The THM models do not provide quantities to other TSPA components, but rather they provide information on the importance of THM effects to the TH and THC models. If these effects are found to be important, they will be incorporated in future revisions of those models.

3.2.2.1 Thermal-Hydrologic-Chemical Drift-Scale Model

The THC drift-scale process model and abstraction are used to determine the incoming (i.e., entering the emplacement drifts) water chemistry and gas-phase composition and flux. The process model is being developed using the TOUGHREACT computer code (the version used will be baselined appropriately), which models chemical reactions and transport of heat, fluid, and solutes. The incoming water composition is a function of the mineral water interactions occurring in the host rock above the emplacement drifts. Relative abundance of participating minerals, equilibrium constants for mineral water reactions, thermodynamic activity coefficients and concentrations of aqueous component species, rate constants (functions of temperature), and reactive surface area all influence precipitation and dissolution rates during heating, which in turn dictate incoming water chemistry. The abstracted water chemistry of interest includes concentrations of constituents important to drip shield, waste package, or waste form degradation, such as Na^+, Ca^{2+}, SiO_2, Cl^-, CO_3^{2-}, SO_4^{2-}, and F^-. The pH also is important, and is influenced by the amount of carbon dioxide (CO_2) available in the gas phase. Other gas-phase components of interest include water vapor (H_2O), oxygen (O_2), and nitrogen (N_2).

The drift-scale THC model is based on an average waste package located at the center of the repository. The drift-scale THC model utilizes lateral symmetry boundary conditions and upper and lower boundary conditions at the ground surface and the water table, respectively.

Specification of mineral abundances, reaction rate constants, surface areas, and other initial conditions are guided, in part, by the results of the drift scale heater test (DST) and the single heater test (SHT) conducted in the ESF (Sonnenthal et al. 1998; Tsang et al. 1999).

3.2.2.2 Multiscale Near-Field and Engineered Barrier System Thermal Hydrologic Model

The multiscale near-field and EBS TH model is used to describe the thermodynamic environment inside the emplacement drifts and the percolation flux above the crown of the drift (which is used to determine the amount of seepage during the thermal period). This model is being developed using the NUFT computer code (the version used will be baselined appropriately), which solves coupled heat and mass-transfer equations. Data needed for the drift thermodynamic environment include drip shield relative humidity and temperature, waste package relative humidity and temperature, temperature at the top of the backfill (or at the drift crown if there is no backfill), and temperature and liquid saturation in the invert. The process-level submodels making up the multiscale near-field and EBS TH model quantify processes such as lateral heat losses associated with proximity to repository edges, spatially and temporally (e.g., because of climate changes) variable infiltration rates, waste emplacement in different host rock units, in-drift heat transfer effects, and waste packages. Therefore, the submodels characterize both large-scale and local-scale heat- and fluid-flow mechanisms. Abstractions of the drift thermodynamic environment (temperature, relative humidity) might be performed for different repository subregions and different waste package types. Determination of appropriate repository subregions could be based on infiltration rate variability, host rock unit, and proximity to repository edge. Determination of appropriate waste package types could be based on time required to return to a specified critical relative humidity for aqueous corrosion or temperature dependence of a specified quantity.

The multiscale near-field and EBS TH model also is used to determine the percolation flux above the crown of the drifts. The percolation fluxes above selected waste package types will be input directly into the abstracted seepage model (Section 3.1) in order to determine the amount of seepage into drifts. The thermal period may include both times of decreased seepage (due to dryout) and increased seepage (due to drainage of thermally mobilized water) compared to ambient. The percolation fluxes obtained from the multiscale near-field and EBS TH model (and thus the resultant seepage) will inherently include the effects of heat-driven water movement, infiltration rate variability, host rock variability, waste package variability, and proximity to repository edges.

The hydrologic property sets applied in the multiscale near-field and EBS TH model will undergo validation and testing using measured temperature results from the DST and the SHT.

3.2.2.3 Thermal-Hydrologic-Mechanical Drift-Scale and Mountain-Scale Models

The THM models that are being developed will actively couple the processes of a TH computer code (TOUGH2) to a TM computer code (JAS3D) (the versions of the computer codes used will be baselined appropriately). The TM model will compute a thermal stress field based on temperature gradients developed during repository heating. The stress field causes mechanical fracture aperture and joint changes. A constitutive model to be developed will relate mechanical alterations to changes in hydraulic properties, and the altered flow properties will be passed to the TH model. Using the mountain-scale model domain developed for the UZ flow and transport model and the near-field model domains developed for the multiscale near-field and EBS TH model, the impact of heat-driven mechanical processes on the evolution of the repository will be assessed. Specifically, mechanical changes in fracture hydrologic properties may alter both large-scale liquid-phase and gas-phase flow fields and percolation fluxes near the crown of an emplacement drift. Furthermore, the impacts of TM processes, such as opening and closing of fractures on the drift thermodynamic environment, will be investigated.

The development of constitutive models that govern mechanical alterations to fracture flow properties are guided by measurements of host-rock displacements taken during the SHT and the DST.

3.2.3 Significant Coupling with Other Models

Climate durations and times of transition (as developed in the UZ flow and transport task), plus the associated infiltrations and water table elevations, are applied to the thermal hydrology and coupled processes. The specific method that would be used depends on whether climate change times are to be sampled within the RIP TSPA code (the version used will be baselined appropriately). In order to vary climate change times from realization to realization within a Monte Carlo simulation, it would be necessary to run the thermal hydrology and coupled processes models separately for each climate state and provide all of them to RIP. Then RIP would switch from one solution to another at the sampled times. On the other hand, if fixed climate change times are used, then the thermal hydrology and coupled processes models would simply incorporate the appropriate climate assumptions.

The hydrologic property data sets developed for the UZ flow model also are applied to the thermal hydrology and coupled processes models. There are calibrated mountain-scale property sets for low, nominal, and high infiltration rates and for flow around and flow through the perched water zones below the repository (Section 3.1). The issue of flow around or through the perched water is not expected to have a significant effect on thermal hydrology, so it may not be necessary to use both sets for thermal hydrology and coupled processes.

The conceptual flow model used for UZ flow and transport is applied to the thermal hydrology and coupled processes models for consistency. The active-fracture dual-permeability model (Liu et al. 1998) is used to describe fluid flow in fracture and matrix continua and flow between the continua. The dependence of the area reduction factor on saturation is an improvement over what was done for the TSPA-VA (CRWMS M&O 1998a, Chapter 2, Section 2.4.3.3) because it allows the fracture-matrix coupling in dryout regions to be different from that in regions with condensate accumulation and drainage.

Thermal hydrology and coupled processes models provide the following information to other TSPA components:

- Temperature and relative humidity at the drip shield and at the top of the backfill (or at the drift crown if there is no backfill) and temperature in the invert for the IDGE
- Water composition of flow above the drift crown for the IDGE
- Gas composition and flux at the repository for the IDGE
- Temperature and relative humidity at the drip shield and the waste package for waste package and drip shield degradation
- Temperature at the waste package for waste form degradation

- Percolation flux above the drift crown for UZ flow and transport (seepage into drifts)
- Liquid saturation in the invert for EBS flow and transport.

3.2.4 Major Assumptions

The following major assumptions apply to the thermal hydrology and coupled processes models for the TSPA-SR. The assumptions will be fully documented and justified in the PMRs or their associated AMRs (aspects of thermal hydrology and coupled processes will be documented in three PMRs UZ Flow and Transport Model; Near-Field Environment Model; and EBS Degradation, Flow, and Transport Model).

- Many of the assumptions listed for UZ flow (Section 3.1) also apply to TH. In particular, assumptions about the dual-permeability flow model, van Genuchten/Mualem saturation-desaturation relations, matrix and fracture hydrologic properties determined by inverse modeling, active-fracture fracture-matrix coupling model, and no small-scale heterogeneity are the same.
- Appropriate values for the chemical kinetics parameters (e.g., reaction rate constants, mineral surface area) are used in the THC models.
- A THC constitutive model can be developed that governs the changes in fracture permeability and fracture capillary pressure based on changes in fracture porosity (changes in fracture porosity are calculated from the amounts of dissolution and precipitation of minerals).
- THM and THC effects can be neglected in the multiscale near-field and EBS TH model. Future applications of the multiscale near-field and EBS TH model (i.e., after SR Revision 0) may include fully coupled THC and abstracted THM (possibly in the form of temperature dependent flow properties), if sensitivity studies show them to be important.
- The multiscale near-field and EBS TH model is an adequate approximation of heat transfer at different scales and the coupling of the scales. Heat transfer assumptions and conceptualizations in the various submodels should be investigated in detail to confirm the adequacy.
- A THM constitutive model can be developed that governs changes in fracture permeability, fracture capillary pressure, and fracture porosity caused by mechanical changes in fracture apertures.

3.2.5 Implementation in Total System Performance Assessment–Site Recommendation

The primary differences in the TSPA-SR treatment of thermal hydrology and coupled processes as compared to the VA (DOE 1998a, Section 3.2) result from changes in the repository design and the UZ flow models (climate, infiltration, and hydrologic properties). Aside from these changes, some additional processes and capabilities are included.

The SR reference design (CRWMS M&O 1999a, Chapter 7) differs from the VA reference design (DOE 1998a, Section 3.2) in a number of important respects. The differences relevant to thermal hydrology and coupled processes are discussed below:

Lower Thermal Load–The areal mass loading has been decreased from 85 metric tons of uranium per acre (MTU/acre) to 60 MTU/acre. A total of 63,000 MTU of CSNF and 7,000 MTU of vitrified HLW and defense SNF are to be emplaced. The nominal loading of 60 MTU/acre includes only the CSNF, implying a loaded area of 1,050 acres. The lower mass loading will result in a cooler repository, on average.

Waste Packages Much Closer Together–Waste packages are line loaded in the drifts, meaning they are placed very close (only 10 cm apart) and form almost a continuous line heat source. The close spacing leads to a strong radiative thermal coupling between the waste packages and tends to reduce waste package temperature variability. Waste packages were much farther apart (up to 10 m) in the VA design (DOE 1998a, Figure 3-18).

Waste Stream Blending–Waste package temperature variability is being reduced even more by blending fuel assemblies in the CSNF waste packages so that initial heat output varies only from about 6 to 12 kW. The VA design did not include blending, and CSNF heat output varied from a few kW to about 18 kW (DOE 1998a, Figure 3-18).

Drifts Much Farther Apart–Drift spacing has been increased from 28 m to 81 m, center-to-center. The drift spacing is determined by the overall areal mass loading and the line-load waste package spacing. The large distance between drifts is designed to prevent coalescence of the boiling zones around adjacent emplacement drifts, thus ensuring that it always will be possible for water to drain between drifts rather than potentially being trapped in a condensation cap above the repository.

Preclosure Ventilation–The reference design now includes a preclosure ventilation period of 50 years, with a forced ventilation rate of 2-15 m^3/s for each emplacement drift. Ventilation will remove heat and moisture from the repository and nearby host rock and will keep peak temperatures lower. The VA design did not include ventilation (DOE 1998a, p. 6-30).

Drifts Backfilled at Closure–Unlike the VA (DOE 1998a, p. 3-31), the new design includes backfill emplaced at the time of repository closure (nominally 50 years after waste emplacement). Backfill material has not yet been specified.

Assumptions about the climate, infiltration, and hydrologic properties are described in Section 3.1.4. As discussed in that section, there are a number of differences between the TSPA-SR analysis and the TSPA-VA (the model and assumptions used for TSPA-VA are described in CRWMS M&O 1998a, Chapter 2, Section 2.4). The thermal hydrology and coupled processes models follow the same hydrologic assumptions as used for UZ flow and transport for consistency.

As in the VA, the majority of the thermal hydrology information is derived from the multiscale near-field and EBS TH model (DOE 1998a, Section 3.2.2.2). The primary output of the multiscale model consists of families of representative time histories of the specified quantities (i.e., temperature, relative humidity, liquid saturation, and percolation flux at various locations).

The families of curves represent variability of conditions, with the variability resulting from spatial variability of infiltration, spatial variability of host rock type, proximity to the repository edges, and variability in waste package heat output. The families of curves for temperature and relative humidity at the waste package and drip shield, and possibly the curves for percolation flux above the drift (converted to amount of water contacting drip shields and waste packages), are used by the waste package and drip shield degradation models to represent spatial variability of environmental parameters. Averages over given repository subregions will also be provided, if needed. The information will be provided for each of the UZ flow cases; that is, three infiltration cases and up to three climate states.

Information on the water and gas compositions and gas-phase flux entering the drifts will be provided by the THC drift-scale model. This model does not have the detailed spatial resolution of the multiscale near-field and EBS TH model (it is expected that only one time history of these quantities will be provided to represent the entire repository). Water and gas composition and gas-phase flux will, however, be provided for each of the UZ flow infiltration and climate cases.

3.2.6 Sensitivity Cases

A majority of the sensitivity cases for thermal hydrology and coupled processes will focus on the coupled process models. The importance of THM and THC coupled processes to repository performance will initially be evaluated by applying a range of assumptions within the existing models. In the longer term, more detailed models are being developed in order to provide a better understanding of coupled processes and a more defensible basis for their effects on the repository. Potential sensitivity analyses with the detailed models are described in the following paragraphs.

THM models are being developed to evaluate the impacts of TM effects on fracture properties in the near- and far-field. Changes in fracture properties (i.e., porosity and intrinsic permeability) due to normal or sheer stresses may influence the flow fields below the repository, the thermodynamic environment within the drifts, and the percolation flux above the drifts. The results of TM and TH model simulations, if found to have a strong impact on repository performance, can be incorporated into other models (e.g., multiscale near-field and EBS TH model, THC drift-scale model) in the form of time- or temperature-dependent functional relationships for fracture porosity, permeability, and other parameters.

THC capability is being developed for the multiscale near-field and EBS TH model. This capability will allow the development of percolation flux and drift thermodynamic environment (i.e., temperature, relative humidity) for different reactive transport processes occurring in the host rock. Consideration will be given to different mineral abundances, ranges of applicable kinetic and thermodynamic parameters and mineral reactive surface areas, and appropriate constitutive relationships governing fracture porosity changes on fracture permeability and other characteristic relations. If found to be important, this information could be included in the multiscale near-field and EBS TH model using a qualified THC version of NUFT (the version used would be baselined appropriately) instead of TH only.

Heterogeneous fracture hydrologic properties in the near-field host rock could be incorporated into the multiscale near-field and EBS TH or THC model to determine the impacts on computed percolation fluxes above the crown of the drift and seepage into the drift. Such analyses could be used to test the seepage abstraction under thermal conditions.

Finally, sensitivity studies associated with repository design may include cases without backfill or consideration of an expanded inventory (e.g., 86,700 MTU of CSNF plus additional HLW and DSNF).

3.2.7 Treatment of Uncertainties

The thermal hydrology models considered in the VA (DOE 1998a, Section 3.2) and other past modeling studies typically have included uncertainties in UZ flow and transport. Infiltration rate uncertainty, hydrologic property uncertainty (including uncertainty in the conceptual flow model), and climate state uncertainty in the TH models have been considered. However, the models have not included uncertainty in thermal properties. With the advent of newer coupled process models, there may be additional important uncertainties. An example of this is the mineral reactive surface area used in the THC calculations. The kinetic rate laws for crystal growth and dissolution of minerals are proportional to the reactive surface area. Variability in the reactive surface area (a highly uncertain parameter) could result in different estimates of fracture sealing by precipitation. This, in turn, could lead to uncertainty in estimated percolation flux above the drift (and therefore uncertainty in seepage) because the percolation flux is proportional to the fracture intrinsic permeability. The effects of THC parameter uncertainty will be investigated in sensitivity cases.

An example of THM parameter and conceptual model uncertainty is in the model predictions for changes in intrinsic fracture permeability. Change in fracture permeability is a function of rock strain, and the rock strain is a function of uncertain rock properties such as thermal expansion, Young's modulus, Poisson's ratio, and fracture frequency and orientation. The importance of the TM parameters and models on hydraulic property changes will be investigated in sensitivity cases.

These coupled-process uncertainties will initially be considered in the TSPA by means of sensitivity analyses. If the uncertainties are found to be important to repository performance, the effects can be included in the TSPA using bounding approximations. In the longer term, when more detailed coupled process models are available, those models will be included directly in the TSPA, if found to be important.

3.3 IN-DRIFT GEOCHEMICAL ENVIRONMENT

The IDGE is defined as the geochemical environment within the emplacement drifts. The IDGE process and abstraction models specifically focus on major element geochemistry and include coupling to seepage and gas entering and leaving the drift, as well as in-drift thermal and hydrologic processes. The purpose of the TSPA-SR IDGE models is to provide a quantitative description of the major time-dependent chemical compositional parameters required by in-drift subsystem models. These subsystem models include the drip shield and waste package degradation models, waste form degradation models, and EBS radionuclide transport model.

This section provides a general description of the IDGE process and abstraction models, major assumptions on which these models are based, and significant couplings between these models and other TSPA models. In addition, this section provides a description of the conceptual model for the TSPA-SR and sensitivity analyses to be performed, and the treatment of important uncertainties in the IDGE.

3.3.1 Introduction

The IDGE component of the TSPA model provides a quantitative description of the changing compositional conditions under which:

- The drip shield and waste package corrodes
- Waste forms degrade and precipitate as secondary phases
- Radionuclides mobilize from the waste form
- Radionuclides migrate through the engineered barriers.

The major compositional changes in the drift are caused by the planned thermal loading of the system (see Section 3.2) and the emplacement of large masses of materials that can react with water and gas (e.g., waste package, waste form, drift liner). Because the system will heat up and then cool off, it will continue to change for several thousand years. The thermal perturbation will affect the movement of gas and water around the emplacement drift, as well as the composition of gas and water in the drift. These perturbed fluids may react with the EBS materials emplaced during repository construction and waste disposal. A schematic of the EBS components in an emplacement drift is depicted in Figure 3.3-1. Most of the EBS components will be very different in chemical composition from the host rock and may alter water and gas compositions before they react with the drip shield, waste package, and waste forms. The EBS components may also provide additional sources of colloids. In addition to these primary effects within the EBS, perturbed fluids generated in the IDGE may react with the host rock as it leaves the EBS. This alteration may change conditions for UZ transport.

Water entering the drift will have variable composition as a result of heating and subsequent boiling and condensation, and reaction of both heated and condensate waters with minerals and gases in the fractures of the host rocks (Wilder 1996; Lichtner and Seth 1996; Hardin 1998). These reacted and thermally perturbed fluid compositions may flow down fracture pathways and enter emplacement drifts, where they may react with EBS materials or boil again and deposit mineral precipitates containing salts. The total amounts of salts deposited within the drifts and on the drip shield and waste package will depend, to some extent, on the composition of ambient water within the UZ. Ambient water compositions measured from the Yucca Mountain SZ within the tuffaceous units (as represented by samples from well J-13) are predominantly dilute sodium bicarbonate fluids with high concentrations of aqueous silica (Kerrisk 1987; Harrar et al. 1990).

In addition to thermally driven perturbations to the flux and composition of water entering a drift, the flux and composition of gas into the emplacement drifts will be affected by the heating of the system (Murphy and Pabalan 1994; Lichtner and Seth 1996: Wilder 1996). One major process affecting the in-drift gas composition is the boiling of the pore water, which is expected to drive most of the air component of the gas out from the drift environment (Murphy and

Pabalan 1994). The changes in the air mass fraction of the gas will drive changes in water chemistry and changes to solid materials in the drifts because of, for example, the interaction of CO_2 gas with water and the resulting change in pH.

Colloids generated from waste forms and steel corrosion products 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 seepage entering the emplacement drifts.

3.3.2 General Description of Process Model and Abstraction

The objective of the IDGE model is to determine the changes in water chemistry resulting from the interaction of EBS materials with water seeping into the drift and to provide this information to TSPA analyses. This model takes into account the variation in seepage and drainage fluxes, the effects of temperature changes on chemical equilibria, and physical processes such as evaporation and condensation.

The IDGE model separates the major potential contributors to water compositional changes into nine subsystem models. These separate models will be used to assess the relative capacities of the different processes to alter compositions of various chemical phases at various times. Such uncoupled models facilitate identification of the processes that may control the bulk chemistry for various time frames. The dominant processes can then be assigned to the appropriate time frames, or the models that need to be coupled can be identified.

The nine subsystem models being developed to represent the IDGE are as follows:

1. **Seepage/Backfill Interactions**–This submodel will evaluate the effect on water chemistry of chemical reactions between water that enters the drift and backfill materials in the drift. The backfill materials may have a mineralogic makeup that is different from the host rock, leading to changes in water chemistry. These changes may affect drip shield, waste package, and waste form performance. Therefore, they will be provided as input to the TSPA drip shield, waste package, and waste form degradation models.

2. **Precipitates/Salts Analysis**–This submodel will determine the types and amounts of precipitates (including salts) that may form as water is boiled within the drift. The submodel will assess the effects on water chemistry of accumulated mass of precipitates, the effect of time and relative humidity on water vapor condensation, and the dissolution of precipitates/salts previously deposited on the drip shield, waste package, and other EBS component surfaces. The evaluation will include changes in concentration of aqueous solutions resulting from evaporation driven by temperature gradients within the drift (e.g., from package surface to drift wall). Mixing of seepage water with this concentrated water will be evaluated in order to determine how much time is required for concentrations to return to ambient levels.

3. **Corrosion Products**–This submodel will evaluate changes to water chemistry resulting from chemical reactions between the aqueous seepage that enters the drift and metallic components and their corrosion products encountered along the flow

paths. These components may include the ground support system, the drip shield, the waste package, the internal waste package structures, the waste package supports, the rail system, and possibly the structural invert materials. Changes to water chemistry due to corrosion products will be provided as input to the TSPA drip shield, waste package, and waste form degradation models. These changes may also affect the transport of radionuclides through the invert and comprise part of the input needed for the EBS radionuclide transport model.

4. **Seepage/Invert Interactions**–This submodel will evaluate the effect on water chemistry of chemical reactions between water that enters the drift and invert materials in the drift. These materials may have a mineralogic makeup that is different from the host rock, leading to changes in water chemistry. Changes in water chemistry due to seepage/invert interactions will be provided as input to the TSPA drip shield, waste package, and waste form degradation models. These changes may also affect the transport of radionuclides through the invert and comprise part of the input needed for the EBS radionuclide transport model.

5. **Seepage/Cement Interactions**–This submodel includes the evaluation of aqueous phase chemical reaction of seepage that has entered the drift with cement initially in equilibrium with the in-drift gaseous phase. Cement may be present in the repository in the form of grout and shotcrete. The potential effects of water/cement reactions on chemical conditions in the drift will be assessed.

6. **In-Package Chemistry**–This submodel provides a quantitative description of the combined effects of important chemical interactions that can occur between aqueous seepage entering the waste package and materials in the package. Materials in the package to be considered include the waste package, the waste package internals, corrosion products from waste package internals, and the waste form.

7. **In-Drift Gas Flux and Composition**–This submodel will assess changes in gaseous phase composition within the emplacement drifts through time arising from the thermal perturbation of the geosphere and reactions of ambient gases with introduced materials. The submodel will include, at a minimum, the concentrations of the following constituents: carbon dioxide, oxygen, nitrogen, and steam. Major processes include the boiling of the water in the emplacement drift and possible chemical interactions between the water, gas, and materials in the emplacement drift that may act as sources, or sinks, for constituents in the gas phase.

8. **Microbial Communities**–This submodel will bound the ultimate abundance of microbes within the drift environment using an approach that evaluates nutrient and energy limitations within the drift. Changes in microbe abundance due to thermal loading and introduced materials will also be considered.

9. **In-Drift Colloids and Concentrations**–This submodel will provide a description of the types of colloids that may result from the introduced materials within the drift, as well as the natural colloids that have entered the drift. Concentrations of these colloid types will be based on stability relations for colloids as a function of the concentration

of dissolved constituents within the water. The constraints on colloid concentrations will be used in the EBS Transport Abstraction model of colloid facilitated radionuclide transport (see Section 3.6). Colloid facilitated transport for plutonium-239 and plutonium-242 will be modeled assuming reversible and irreversible attachment.

The relationships between submodels, their coupling, and spatial locations of potential importance are illustrated schematically by a series of mixing cells that represent the key spatial locations within an emplacement drift (see Figure 3.3-2). In this figure, five spatial domains are identified:

1. The backfill region above the drip shield.
2. The drip shield environment, defined as the backfill region immediately on or adjacent to the drip shield.
3. The waste package environment, defined as the region immediately on, or adjacent to, the waste package (this region may, or may not, include backfill, invert, or corrosion products).
4. The waste form environment, which includes the interior of the waste package.
5. The EBS transport pathway environment, which includes the region underneath and between the waste package and drift wall.

The dashed lines in the figure indicate that the subprocess is likely to be of minimal importance in the indicated spatial domain. When more than one subprocess occupies a box, there is potential for the subprocesses to be coupled within the spatial domain.

Coupling between the various subprocesses and mixing cells can be achieved by identifying conceptual scenarios that link flow through mixing cells along a flow pathway. These pathways can be examined both with and without a particular subsystem model included in a cell as a means to assess the importance of the corresponding subprocess. Figure 3.3-3 illustrates a conceptual scenario that includes five mixing cells connected by seepage fluxes that transport dissolved chemical components from one cell to another. Cell-to-cell liquid fluxes for this model will be abstracted from the EBS Water Distribution and Removal model and the EBS Physical/Chemical Environment Model, which are described in Section 3.6. In this scenario, the seepage entering the drift flows downward through the backfill (Cell 1) and contacts the drip shield. The drip shield diverts a major fraction of this seepage, and the remaining fraction penetrates the drip shield through breaches. The diverted seepage is shown to bypass diverted Cells 3 and 4 and flow into the invert (Cell 5). Similarly, a fraction of the flux penetrating the drip shield enters the breached waste package and the remaining fraction flows into the invert (Cell 5). This figure depicts one of many possible scenarios. Other scenarios involving different flow paths and repository representations are possible, depending on the EBS design and objective of the analysis (e.g., it may be appropriate in some cases to simplify the drift representation and combine the drip shield and waste package cells into a single drip shield/waste package cell). Also, only one cell would be required if the focus of the analyses is to examine one particular aspect of the system, such as seepage/waste-form interactions. The implementation of results from these analyses within RIP is discussed below. For additional discussion on SR analyses, refer to Sections 3.3.5, 3.3.6, and 3.3.7.

The flow through mixing cells will be linked together using the Geochemical Repository Integration model (GRIM) software package. The subprocesses and evolution of water in each mixing cell will be evaluated using the EQ3/6 software package with the solid-centered flow through capability. GRIM tracks the seepage flow through each cell and transports the cell's effluent to downstream cells according to the prescribed flow paths; altered solids remain in each cell for reaction at subsequent times. GRIM affords the following key advantages over the approach used in the TSPA-VA:

- It facilitates data traceability, data consistency, and output data reproducibility.
- It explicitly couples in-drift seepage flux with reaction processes.
- It allows assessment of a range of conditions.
- It provides time-dependent output of key variables that describe the waste package, waste form, and radionuclide transport environments.
- It allows assessment of the effects of coupled chemical processes on drip shield/waste package, and radionuclide transport environments.

The scenario shown in Figure 3.3-3 represents a complex problem that includes a mixing cell for each of the key regions in an emplacement drift. The complexity of this problem increases further, depending on the number of subprocesses included in each cell. Process level IDGE analyses for the SR will rely on a combination of bounding analyses and simplified one or two cell representations involving a limited number of subprocesses. For further discussion on SR analyses, refer to Sections 3.3.5, 3.3.6, and 3.3.7.

The nine submodels listed previously will be grouped into three IDGE model abstraction components:

1. A component for water-solids-gas chemistry (submodels 1 through 7).
2. A component dealing with the influence of microbial environments.
3. A colloid concentration component.

The primary model affecting the TSPA representation of the EBS is the water-solids-gas component. The primary products of this component will be time-dependent bounds on the ranges of dissolved constituents that are needed as inputs (e.g., pH, Cl^-, F^-, SiO_2, CO_3^{2-}, Ca^{2+}, Na^+, and SO_4^{2-}) to drip shield and waste package corrosion, waste form degradation, and solubility limited radionuclide concentration analyses. Results from the microbial communities component will be used for a bounding analysis to evaluate microbial effects on water chemistry and transport, and will not feed directly into the other components. The colloid component will use solution ionic strength, as provided by the water-solids-gas component, to determine the concentration of colloids in solution. The concentration of colloids in solution, in conjunction with the assumption of reversible and irreversible sorption, will be used to calculate releases of colloidal plutonium from the EBS.

Results of the water-solids-gas chemistry abstraction component will be abstracted EBS fluid composition response surfaces for various regions of the EBS. These response surfaces will set the chemical environment within the RIP EBS cells. Each RIP EBS cell is an equilibrium batch reactor that has advective and diffusive components of transport into and out of the cell. By coupling time histories of IDGE compositional parameters to each cell environment, the IDGE model will be effectively coupled to the waste form degradation model, waste form mobilization model, and EBS transport model. Hence, the basic modeling approach is to provide response surfaces from the IDGE model to the various RIP EBS cells.

3.3.3 Significant Coupling with Other Models

The IDGE model has several connections with other TSPA component models. This model takes input from the UZ flow and thermal hydrology models and provides output to the drip shield and waste package corrosion models, the waste form model (degradation, radionuclide mobilization, and EBS transport), and the UZ radionuclide transport model. The connections are discussed in more detail below.

Unsaturated-Zone Flow–The flux of water and dissolved constituents in the IDGE is given either as the seepage flux through the drifts or as the average percolation flux at the repository horizon. Seepage flux is used for the in-drift water solids model and the colloid model. Average percolation flux is used for the in-drift gas model, because gas mobility is relatively high near the drifts. Therefore, the gas composition is in equilibrium with a much greater volume of water than just the seeping water.

Thermal Hydrology–The thermal disturbance caused by repository heating provides a number of time-dependent boundary conditions for the IDGE model. These conditions include the flux of groundwater and gas into the drift, the drift temperature, and the relative abundance of air in the gas. Thermal effects can drive changes in the fluid and gas compositions through changes to temperature dependent phase equilibria or reaction kinetics. Such changes may also occur within the heated host rock surrounding the EBS and change the compositions of those incoming phases. The effects of thermal perturbations may also have long-term consequences for minerals and solids within the drift because of changes in phase stabilities, reaction rates, permeabilities, and porosities.

Drip Shield and Waste Package Degradation–The in-drift geochemistry may impact the corrosion of the drip shield and waste package barrier materials. The composition of water contacting the drip shield and waste package, and the bulk oxidation state within the drifts, are supplied by the IDGE model. Also, just as drip shield and waste package degradation will be affected by the composition of fluids reacting with them, the drip shield and waste package materials themselves are an extensive mass of introduced materials. These materials and their solid corrosion products may change the aqueous and gas compositions in the drift, as well as provide a source of iron oxyhydroxy colloids that may enhance migration of certain radionuclides.

Waste Form Degradation, Mobilization, and Engineered Barrier System Transport–The degradation rates of the waste forms, including cladding, depend on the composition of the gas phase and the aqueous phase reacting with the waste form, as well as other factors, such as mechanical loads. The IDGE component provides the compositions of water and gas that may react with the waste forms and provides the state of materials through which radionuclide transport will occur in the EBS. The major chemical constituents of the waste form have also been evaluated for their potential to change the water chemistry from its initial composition.

Unsaturated Zone Radionuclide Transport–The overall composition of the water that moves from the EBS into the UZ transport pathway is determined from the IDGE component model. Radionuclide transport depends on water composition, particularly for radionuclide retardation processes, but also for potential alteration of the pathways themselves. The potential altered fluid compositions that may migrate through the UZ will be used as constraints on sensitivity analyses of coupled processes in the unsaturated zone.

3.3.4 Major Assumptions

The IDGE model takes input from the UZ flow and thermal hydrology components and provides output to the drip shield and waste package degradation models, the waste form degradation model, and the EBS radionuclide transport model. Like the overall TSPA model, the IDGE model is based on the assumption that thermal, hydrologic, and chemical processes can be decoupled, calculated separately, and linked. This assumption permits the IDGE model, other in-drift subsystem models, and TSPA components to be linked in a single direction via output/input transfers at the process model level, or by one-way, direct connections within the TSPA analyses. In addition to the major assumption that thermal, hydrologic, and chemical processes can be decoupled, the following key assumptions apply:

- An emplacement drift can be represented by a set of discrete mixing cells that represent key spatial domains in the drift, e.g., mixing cells may be linked to represent the following spatial domains:
  - The backfill region above the drip shield
  - The backfill region immediately adjacent to the drip shield or waste package
  - The interior of the waste package
  - The region immediately underneath the waste package
  - The region containing the invert.
- The transport into and out of a mixing cell is advection dominated.
- The composition of the in-drift gas phase is homogeneous; this is assumed because of rapid migration of gas constituents at the drift scale. This assumption precludes generation of local changes to the in-drift gas composition from a reaction with materials that are abundant compared to the masses of available gas phase constituents, such as oxygen and carbon dioxide. This assumption is robust because gaseous diffusion alone is rapid enough to ensure homogeneity at the drift scale.

- Reaction between water and solids in the drift and waste package occur at gas fugacity and flux conditions derived from the in-drift gas flux and composition model.

- Water movement through the drift is slow compared to the reaction rates between the water and solids in the drift. Therefore, reactions proceed to equilibrium.

3.3.5 Implementation in Total System Performance Assessment–Site Recommendation

The IDGE abstraction model results will be used by the drip shield and waste package degradation models (see Section 3.4), the waste form degradation model (see Section 3.5), and the radionuclide transport model (see Section 3.6). These subsystem models will be implemented in TSPA-SR by either directly linking or abstracting to the RIP model. Within RIP, IDGE results will be used to set the variables for water and gas composition, and solid phases as a function of time.

The TSPA-SR IDGE model will include the following aspects:

- The uncertain quantities and compositions of seepage and gas entering the emplacement drift will be provided to the IDGE abstraction model as input within RIP. This information will be developed using UZ reactive transport process model calculations and abstracted to RIP (for discussion of these uncertain quantities, refer to Sections 3.1 and 3.2).

- The important IDGE chemical compositional parameters within the drift will be a function of the uncertain quantities and compositions of seepage and gas entering the emplacement drift. In the VA, important compositional parameters within the drift were calculated for the mean-value deterministic case only. The new approach will permit direct incorporation of drift boundary condition uncertainties into the TSPA RIP calculations.

- Spatial variability in the IDGE will be included, both within the drift and between repository regions. To account for in-drift variability, response surfaces for compositional variables will be developed for the following locations drip shield surface, waste package surface, waste form surface, interior waste package surface, and in the invert.

- A bounding assessment of the effects on water chemistry of accumulated precipitates (including salts) that may form as water evaporates in the drift will be included. The time and relative humidity controls on water vapor condensation, and the dissolution of precipitates/salts previously deposited on the drip shield and waste package, will also be included. The drip shield and waste package degradation abstraction models will use this information.

- Response surfaces will be developed based on calculations that explicitly couple chemical reactions to water flow.

Key inputs to the IDGE calculations will include (1) a set of initial materials within the model emplacement drift and waste package and their major element composition and thermodynamic/kinetic coefficients, (2) time-dependent water and gas fluxes into the drift provided by the drift seepage calculations, (3) time-dependent compositions of incoming water and gas entering the drift provided by the drift seepage composition calculations, (4) in-drift temperatures provided by the results of the TH calculations, and (5) abstracted in-drift water fluxes (including fluxes into the waste package) and saturation provided by the EBS Water Distribution and Removal Abstraction Model and the EBS Physical/Chemical Environment Model.

3.3.6 Sensitivity Cases

A series of sensitivity analyses will be conducted to evaluate the potential impact of specific chemical processes and uncertain data inputs on estimates of important compositional parameters required by the EBS subsystem models and radionuclide releases from the EBS. A preliminary list of sensitivity analyses is provided below.

- Bounding assessments on microbial community development will be conducted to provide an assessment of potential changes to both in-drift gas and fluid compositions. If these changes appear to be potentially significant relative to the abiotic chemistry, then they will be directly incorporated into the water-solids-gas chemistry model.

- The effects on water chemistry of chemical reactions between water that enters the drift and backfill materials in the drift that are different from the host rock will be evaluated. If changes in water chemistry are found to have a potentially significant impact on radionuclide releases from the EBS, then these reactions and their effects on water composition will be explicitly incorporated into the water-solids-gas chemistry model.

- The effects on water chemistry of chemical reactions between the aqueous seepage that enters the drift and metallic components and their corrosion products encountered along the flow paths within the drift will be evaluated. If changes in water chemistry are found to have a potentially significant impact on radionuclide releases from the EBS, then these reactions and their effects on water composition will be explicitly incorporated into the water-solids-gas chemistry model.

- The effects on water chemistry of chemical reaction between seepage that has entered the drift with cement initially in equilibrium with the in-drift gas will be evaluated. Potential effects of water/cement reactions on chemical conditions in the drift will be assessed, factoring in the influence of carbonation and different seepage rates and compositions. If changes in water chemistry are found to have a potentially significant impact on radionuclide releases from the EBS, then these reactions and their effects on water composition will be explicitly incorporated into the water-solid-gas chemistry model.

- The effects on water chemistry of chemical reactions between water that enters the drift and invert materials in the drift different from the host rock will be evaluated. These changes may affect the transport of radionuclides through the invert. If changes in water chemistry are found to have a potentially significant impact on radionuclide releases from the EBS, then these reactions and their effects on water composition will be explicitly incorporated into the water-solids-gas chemistry model.

3.3.7 Treatment of Uncertainties

The two major sources of uncertainties in the IDGE are conceptual model uncertainties and, to a lesser degree, parameter uncertainties. The general approach to conceptual model uncertainty in the IDGE is to separate the major potential contributors to water compositional changes into various subsystem models (e.g., seepage and cement interactions, in-package chemistry, in-drift gas flux and composition). These separate models will be used to individually assess the relative potential of each process to alter composition in the drift during postclosure. This approach will facilitate identification of processes that may control the bulk chemistry for various time frames. These dominant processes can then be assigned to the appropriate time frames and the models that should be coupled can be identified.

Parameter uncertainty arises from two main sources. The first important source is uncertain emplacement drift boundary conditions (e.g., water seepage and gas fluxes into the drift and their composition) during the postclosure period. These boundary condition uncertainties will be captured in the probabilistic TSPA, as described in Sections 3.1 and 3.2. The propagation of these uncertainties through the IDGE models will be represented by calculating IDGE conditions within RIP that are specific to each set of sampled (uncertain) seepage and gas fluxes and their composition. This approach will involve the application of IDGE process based response surfaces that will be developed for a range of emplacement drift boundary conditions, spanning their potential uncertainty range. Then, the IDGE system responses for a specific set of boundary conditions (e.g., pH on the drip shield surface and pH at the waste form surface) will be interpolated from response surface functions for these quantities.

The second source of parameter uncertainty is uncertain thermochemical data (e.g., equilibrium constants and kinetic rate constants). The potential impact of the uncertainties will be accounted for by implementing bounding approaches whenever possible, e.g., to account for uncertainty in the kinetic reaction rate for oxidation of chromium, it may be assumed that chromium in the stainless steel components of the waste package internals will oxidize fully to chromate (or dichromate) on the time scale of interest. However, laboratory observation of the corrosion of chromium containing steels and alloys indicate that such oxidation may be extremely slow. Therefore, the assumption of full oxidation is conservative in the sense that it will enhance acidification of in-package seepage, which will increase degradation of CSNF in some cases.

3.4 WASTE PACKAGE AND DRIP SHIELD DEGRADATION

The waste package is a primary component of the EBS defined by the NRC in proposed 10 CFR 63.2 (64 FR 8640) to include the following:

- The container
- The waste form (e.g., CSNF, defense HLW, defense SNF)
- Shielding (if used), packing, or other absorbent materials immediately surrounding the waste form.

As with the reference design in the VA (DOE 1998a), the current waste package design (CRWMS M&O 1999a) consists of dual walls; however, in the SR design, the outer wall is made of corrosion resistant material (CRM) with the inner wall material selected to provide structural support. In the SR design (Figure 3.3-1) the waste package (using the NRC definition) for the CSNF has four distinct barriers (listed from the outside in):

- 2 cm thick Alloy-22 outer wall
- 5 cm thick stainless steel (316NG) inner wall
- Fuel rod cladding (typically made of a zirconium-alloy metal)
- SNF (i.e., uranium oxide ceramic pellets that have been used in a nuclear reactor).

A drip shield is also an integral part of the current EBS design (Figure 3.3-1) and serves to divert water entering the drift, and thus, preventing water from dripping onto the waste package. The drip shield is to be made of 2 cm of Alloy Grade-7 titanium. In addition, the use of a backfill material (at the time of closure) is part of the EBS design. The backfill would provide an additional barrier that would serve to prevent waste package damage by rockfalls, as well as contribute to controlling radionuclide releases from the EBS (see Sections 3.6 and 4.7 for more detailed descriptions).

The waste package and drip shield will play a very important role in containing waste in the repository for tens of thousands of years. Regarding postclosure isolation performance, the waste package has been specifically designed to achieve the following:

- Confine the nuclear waste within the repository for tens of thousands of years
- Provide a combination of engineered barriers that will protect the waste form from the in-drift environmental conditions and degradation processes (e.g., by diverting advective water flow around the waste)
- Limit the radionuclide release to the UZ.

It is important to note that the waste package will also serve a number of important preclosure performance functions during the 50 year (or longer) operational period, which will not be discussed here.

The purpose of the waste package and drip shield process level models and abstraction is twofold. First, the waste package and drip shield models are intended to provide tools for developing a detailed understanding of the corrosion modes (e.g., general and localized corrosion) affecting the waste package and drip shield and their dependence on in-drift environmental conditions (e.g., temperature, relative humidity, seepage flow rate, water chemistry) that vary with time and location in the repository. Second, the waste package model provides estimates of the service life (referred to as waste package lifetime) on a probabilistic basis. The waste package lifetime (or failure time) is conservatively defined as that length-of-time from repository closure until the first perforation (i.e., the first complete pit penetration, first crevice propagation, or first patch opening through the two container walls). The drip shield lifetime is similarly defined as the length of time before the drip shield is perforated. In the case of the waste package, it is important to note that even after failure, water flow through the dual wall waste package will be limited by the geometry of perforations. Thus, a perforated waste package could provide significant resistance to water ingress and, in turn, effectively control or constrain radionuclide release rates to the UZ.

The purpose of this section is to provide the technical basis for the waste package and drip shield process models including the conceptual framework and key assumptions. In addition to calculating the waste package and drip shield performance attributes for the TSPA-SR base case, the process level models and abstractions will also be used in sensitivity analyses to gain further insight into factors affecting multiple barrier performance.

3.4.1 Introduction

The process level model for the waste package has been evolving over the past decade as a result of an improved knowledge base, but also because of design changes in the waste package and EBS (CRWMS M&O 1999a). For example, since publication of the VA (DOE 1998a), the waste package design has changed from a dual wall container with an outer corrosion allowance material (CAM) and inner CRM to a design with the CRM on the outside and CAM on the inside. Another important evolution of the waste package model is that premature failures (caused by manufacturing or material defects) were previously treated as an initial condition. Now they will be modeled on a mechanistic basis. Also, the drip shield and backfill are completely new components of the EBS and are now accounted for in the waste package process level model.

3.4.2 General Description of Process Model and Abstraction

In the new reference design (CRWMS M&O 1999a), the approximately 10,000 waste packages would be placed end-to-end (emplacement strategy known as line load) in the mined drifts. Some of the design features that are significant to the process level models and abstraction include:

- Drift diameter of 5.5 m
- Invert of steel, with sand or gravel ballast
- Drift center-to-center spacing of 81 m
- Areal mass loading of 60 MTU/acre
- Preclosure ventilation (e.g., 2-15 m^3/s airflow, depending on duration of ventilation) |

- Drip shield, consisting of 2 cm titanium Alloy Grade-7 (titanium-7)
- Backfill: granular material.

A primary objective of the waste package model is the estimation of waste package lifetime. The conceptual model describes the natural degradation (general and localized corrosion) of the container and drip shield to environmental conditions in the emplacement drift. Of key importance to the degradation rate are the factors that make up the localized environmental conditions consist of such conditions as:

- Relative humidity

- Temperature (i.e., at the waste package surface)

- In-drift gases (e.g., H_2O, O_2, CO_2, N_2)

- Chemistry of water and mineral films on the waste package (e.g., precipitates, salts, and pH)

- Presence (or absence) of water dripping on the waste package surface.

Most of these environmental conditions, which are induced by heat transfer caused by the waste package decay heat, are also important factors to the barrier performance of the drip shield.

Within the process level models for the waste package and drip shield, the characteristics of the degradation modes are to be quantitatively evaluated. Output from these process models—essentially the rates of degradation for each of the degradation modes—are to be used by modules of the WAPDEG (CRWMS M&O 1998b; 1999b) computer code to determine longevity and subsequent degradation area for the waste package and drip shield. In this regard, WAPDEG should be considered the abstraction of the degradation process models.

The degradation processes that are expected to be considered for TSPA-SR are as follows.

- Humid air corrosion
- General aqueous corrosion
- Crevice corrosion
- Pitting corrosion
- Stress corrosion cracking
- Hydride cracking
- Long-term phase stability.

A submodel for each of these processes will be developed and incorporated into WAPDEG unless the impact of the process is found to be insignificant to waste package/drip shield degradation (i.e., the version of WAPDEG used for TSPA-SR will be as simple as possible, while still capturing the significant effects on performance). Not all the above processes will be considered in equal detail. Processes that are expected to be most important to performance and have available data associated with them will be developed in the most detail. For example, localized corrosion might be a more significant failure mechanism than general corrosion over a 10,000-year period for corrosion resistant metals, and thus would be modeled in more detail.

Dry oxidation of the waste package and the drip shield is not expected to be considered in TSPA-SR. This process has been found to be insignificant in the degradation of corrosion resistant metals, such as Alloy-22 and titanium-7, in previous analyses. Also, direct damage from rockfall will not be considered as long as the repository design includes backfilling the drifts. Also, microbial influenced corrosion will not be considered directly, since it is not expected to have much effect on the current waste package design. However, as mentioned in Section 3.3, there will be sensitivity analyses to support this assumption.

A basic objective of the new reference design (CRWMS M&O 1999a) is to produce a waste package that contains the radioactive waste for a period of 10,000 years or longer. As testing data for the reference design becomes available, it is expected that the combination of drip shield and waste package will be shown to meet this goal in future performance assessment analyses. That is, TSPA-SR should not forecast releases of radionuclides during a 10,000-year performance period if the repository evolves as designed. Thus, the combination of a drip shield and waste package failure during this period is anticipated to be a rare event (e.g., a premature failure caused by defects in materials or manufacturing, or by unexpectedly rapid corrosion due to unanticipated environmental conditions). The aim of TSPA-SR is to model the progression of defects to complete failure on a mechanistic basis, where possible. In order to evaluate the impact of these relatively low probability events, measures will be taken in TSPA-SR to determine their probability of occurrence and their consequences, perhaps separately from the Monte Carlo simulations used in TSPA calculations.

The WAPDEG computer code will contain modules to simulate the evolution and transition of the individual degradation processes over a given number of representative drip shield and waste package pairs in various locations in the repository. Also, the surface of each drip shield and waste package will be subdivided into regions (patches) where the degradation is calculated independently. In this manner, the variability of the degradation over the repository and over each drip shield and waste package will be accounted for (Section 3.4.6). Environmental conditions will be input from other TSPA components, including UZ flow (seepage), thermal hydrology, and IDGE (Section 3.4.3). It is planned to couple WAPDEG directly with the TSPA computer code, RIP, to facilitate traceability and consistency of parameter values between the waste package degradation component and other TSPA component models.

3.4.3 Significant Coupling with Other Models

The performance of the waste package and drip shield is strongly coupled and dependent on the evolution of the in-drift conditions. Specifically, the various modes of general and localized corrosion are a strong function of:

- Hydrothermal conditions (temperature, relative humidity)
- Chemical composition of gases (H_2O, O_2, CO_2, N_2), dripping water (pH, etc.), and mineral deposits (precipitates and salts)

- Hydrologic conditions (seep flow rate and seep patterns).

In addition, the waste package/drip shield models may also be coupled to the disruptive scenario models (e.g., rockfall, igneous intrusion or extrusion, and faulting) if it is found necessary to determine waste package and drip shield lifetimes under these conditions.

For the TSPA-SR, various process level models will be run to produce simulations of the in-drift environmental conditions and their evolution over the regulatory time period of 10,000 years per proposed 10 CFR 63 (64 FR 8640). The thermal hydrology component of TSPA (Section 3.2) will define the hydrothermal conditions in the vicinity of the waste package, and will produce the temperature and relative humidity histories at representative locations within the repository footprint. Similarly, the TSPA component for the IDGE will generate a range of gas and liquid compositions (Section 3.3). Drift scale simulations of the hydrologic conditions will be performed by the unsaturated-zone flow component (Section 3.1).

Simulation results of in-drift environmental conditions (generated with the process level computer models) will be abstracted into lookup tables. These will be used in the waste package and drip shield model abstraction implemented in an updated and qualified version of the WAPDEG code used in the VA (DOE 1998a, Volume 3, Section 3.4.2).

3.4.4 Major Assumptions

The WAPDEG model for the waste package and drip shield degradation is built on a modeling approach that utilizes stochastic representations of (1) general and localized corrosion mechanisms, (2) temporal and spatial evolution of THC conditions on waste package and drip shield surface, and (3) effects of materials and manufacturing defects and long-term aging and phase stability of the waste package and drip shield. For the conceptual models implemented in the waste package model, the following generic assumptions apply:

- There will be no corrosion of drip shield and waste package during the preclosure ventilation period (i.e., for 50 years or longer). This is based on the rationale that during that period, there will be no drips onto the waste package and drip shield, and the relative humidity at the waste package and drip shield surfaces will be low.

- The drip shield and backfill are emplaced at the time of repository closure (i.e., after 50 years or later).

- Waste package and drip shield corrosion initially occurs from the outside inward. That is, corrosion of the inner wall of the waste package occurs only after complete perforation (i.e., pits or cracks) of the outer wall.

- When the condition of dripping on the waste package or drip shield occurs, the amount of area wetted by drips is variable and can be represented by random sampling over a given range. Salts and potentially aggressive water chemistry develop only on those wetted areas. The critical relative humidity above which stable water film can form on the wetted area will be dependent on the type of salt forming.

- The wetted area on the waste package and drip shield from drips will have 100 percent probability of crevice formation. This conservative assumption is employed because of a large uncertainty associated with the characterization and quantification of salts and mineral scales that potentially form crevices on the wetted area.

- Only the closure welds of waste package will be subject to SCC. This is because tensile stress is required for crack growth.

- For the areas on the waste package and drip shield that are not affected (or not wetted) by drips, the stable water film needed to initiate aqueous corrosion will form from the condensation of water vapor in the drift. The surface of the waste package and drip shield in the emplacement drift is contaminated (or covered) with dirt and debris from various repository operations including waste package, drip shield, and backfill emplacement operations. Because those particles will provide sites for capillary condensation of water, water film can form on the waste package and drip shield surface at humidities below the saturated vapor pressure.

- As long as the drip shield is not perforated, the contact points between the waste package outer barrier and the waste package supports, and those between the waste package outer barrier and drip shield inner surface do not result in aggressive crevice conditions. This is based on the rationale that the presence of aggressive species such as chloride ions is required to initiate crevice corrosion of the alloys comprising the waste package outer barrier and drip shield. The condensed water that forms at the contact points while the drip shield is unbreached will lack such aggressive species.

- As the waste package support degrades, the waste package will settle down onto the floor of the emplacement drift. When this happens, the bottom of the waste package will contact the invert materials and seepage water. These could potentially result in crevice corrosion attack on the bottom of the waste package outer barrier.

- Spatial and temporal variability in waste package and drip shield corrosion processes (corrosion initiation and penetration rate) will be represented by explicitly incorporating spatial and temporal variations of the exposure conditions in the repository (i.e., temperature, relative humidity, and water chemistry at the waste package and drip shield surface).

- Spatial variability in corrosion processes within a waste package and drip shield will be represented by randomly populating relevant corrosion process parameters (such as area wetted by drips, corrosion initiation and penetration rate) over the subareas (referred to as patches) on the waste package and drip shield surfaces.

Several of these assumptions will be investigated further for appropriateness before TSPA-SR analyses (also see Section 3.4.6).

3.4.5 Implementation in Total System Performance Assessment–Site Recommendation

For the purposes of the TSPA-SR, the conceptual model for the waste package and drip shield will be constrained by the coupled processes that control the progression of barrier material degradation (in response to the exposure conditions in the EBS) (see Section 3.4.2). The in-drift exposure conditions for the nominal scenario constitute the expected FEPs for the EBS (Section 2.2). This category of FEPs (or driving forces) are primarily associated with climatic changes (projected for the regulatory period and beyond) and the TH regime, generated by decay heat. Excluded from the base case are waste package and drip shield degradation and failure modes attributed to disruptive FEPs (i.e., scenario classes such as igneous activity and faulting).

The conceptual model is based on a discretized representation of the waste package and drip shield component geometries. This approach, which was specifically chosen to capture realistically the spatial variability of corrosion rates, consists of subdividing waste package and drip shield surfaces into rectangular grids, or patches, as illustrated in Figure 3.4-1. Within each patch, the effects of localized and general corrosion are modeled as a function of the temporally and spatially evolving exposure conditions, such as:

- Dripping and nondripping conditions (associated with in-drift seepage)
- Water and gas compositions and chemical properties (e.g., pH, f(O_2))
- Temperature and relative humidity conditions
- Formation of salt deposits and concentrated salt solutions (Cl^-).

The susceptibility to degradation by localized corrosion processes of the CRMs for the waste package and drip shield (i.e., Alloy-22 and titanium-7, respectively) is higher in the presence of high salt concentrations. Some of the patches on the waste package/drip shield surface may not be subject to water dripping or attendant salt layer formation. In this case, the dominant degradation process would be humid air corrosion, which is a very gradual process, even over time periods of 10,000 years.

The conceptual model for TSPA-SR is being implemented in a new version of WAPDEG computer code. The specific degradation processes and the associated model parameters are listed in Table 3.4-1. The new version of WAPDEG is expected to use more mechanistic representations of corrosion processes. It will be supported by qualified data and recent corrosion test data relevant to site-specific conditions. The new version of WAPDEG will treat the propagation of uncertainty and spatial variability in a more comprehensive manner (Section 3.4.7).

Results of analyses produced with the WAPDEG code will be a quantitative assessment of waste package and drip shield performance. The WAPDEG output will be presented as a time-to-first-breach of the waste packages and drip shields. The form will be of small holes (pits or cracks) or slightly larger holes (crevices) resulting from localized corrosion. Subsequent perforations (or openings) of the breached waste packages and drip shields will be determined as a function of time, giving a measure of the perforation area available for transport of radionuclides out of the package. General corrosion, which results in larger openings, is not expected to be important during the first 10,000 years after closure.

Table 3.4-1. Summary of Degradation Processes and Their Parameters to be Included in the Conceptual Model Waste Package and Drip Shield Degradation Analysis for TSPA-SR

Processes/Topics	Parameters
Evolution of Exposure Condition on Waste Package Outer Barrier and Drip Shield	Chemistry of Water Film on Waste Package and Drip Shield Surface in the Presence and Absence of Dripping
	Temperature and Relative Humidity Thresholds for Aqueous Corrosion Initiation of Waste Package Outer Barrier and Drip Shield
	Chemistry of Water at the Interface Between Waste Package Outer and Inner Barriers After Outer Barrier Breach
	Uncertainty and Variability of Corrosion Initiation Thresholds for Waste Package Outer Barrier and Drip Shield
General Corrosion of Waste Package Outer Barrier and Drip Shield	General Corrosion Rate Of Alloy-22 Outer Barrier and Drip Shield in the Presence and Absence of Dripping
	Penetration Opening Size (or Patch Size) Distribution
	Uncertainty and Variability of Alloy-22 Outer Barrier and Drip Shield General Corrosion Rate
Pitting and Crevice Corrosion of Waste Package Outer Barrier and Drip Shield	Pitting Corrosion Initiation Threshold for Alloy-22 Outer Barrier and Drip Shield
	Crevice Corrosion Initiation Threshold for Alloy-22 Outer Barrier and Drip Shield
	Probability of Crevice Formation on Alloy-22 Outer Barrier and Drip Shield in the Presence of Dripping
	Pit Density Distribution on Alloy-22 Outer Barrier and Drip Shield
	Crevice Density Distribution on Alloy-22 Outer Barrier and Drip Shield
	Pitting Corrosion Rate of Alloy-22 Outer Barrier and Drip Shield
	Crevice Corrosion Rate of Alloy-22 Outer Barrier and Drip Shield
	Effect of Phase Stability and Thermal Aging on Alloy-22 Outer Barrier Pitting and Crevice Corrosion Initiation and Corrosion Rate
	Pitting and Crevice Corrosion Penetration Opening Size Distribution on Alloy-22 Outer Barrier and Drip Shield
	Uncertainty and Variability of Pitting and Crevice Corrosion Initiation Thresholds and Corrosion Rate of Alloy-22 Outer Barrier and Drip Shield
SCC of Waste Package Outer Barrier and Drip Shield	SCC Initiation Threshold for Alloy-22 Outer Barrier and Drip Shield
	SCC Penetration Rate of Alloy-22 Outer Barrier and Drip Shield
	Effect of Phase Stability and Thermal Aging on Alloy-22 Outer Barrier SCC Initiation and Penetration Rate
	SCC Crack Opening Size Distribution on Alloy-22 Outer Barrier and Drip Shield
	Uncertainty and Variability of SCC Initiation Thresholds and Rate of Alloy-22 Outer Barrier and Drip Shield
HIC of Drip Shield	HIC Initiation Threshold for Drip Shield
	HIC Penetration Rate of Drip Shield
	HIC Crack Opening Size Distribution on Drip Shield
	Uncertainty and Variability of HIC Initiation Thresholds and Rate of Drip Shield

Table 3.4-1. Summary of Degradation Processes and Their Parameters to be Included in the Conceptual Model Waste Package and Drip Shield Degradation Analysis for TSPA-SR (Continued)

Processes/Topics	Parameters
Corrosion of 316 Stainless Steel Inner Barrier	Chemistry of Water at the Interface Between Waste Package Outer and Inner Barriers After Outer Barrier Breach
	General Corrosion Rate of Inner Barrier Underneath Breached Alloy-22 Outer Barrier
	Pitting and Crevice Corrosion Threshold and Penetration Rate of Inner Barrier Underneath Breached Alloy-22 Outer Barrier
	SCC Initiation Threshold and Penetration Rate of Inner Barrier Underneath Breached Alloy-22 Outer Barrier
	Penetration Opening Size Distribution in Inner Barrier from General Corrosion, Pitting and Crevice Corrosion, and SCC
	Uncertainty and Variability of the Interface Corrosion Chemistry and General Corrosion Rate
	Uncertainty and Variability of Pitting and Crevice Corrosion Initiation Thresholds and Penetration Rate
	Uncertainty and Variability of SCC Initiation Threshold and Rate
Effects of Material and Manufacturing Defects, Mechanical Stress, and Other Nonconventional Degradation Processes	Effect of Material and Manufacturing Defects on Initiation and Penetration Rate on Pitting Corrosion, Crevice Corrosion, SCC, and HIC (Drip Shield Only) of Alloy-22 Outer Barrier and Drip Shield
	Effect of Phase Stability and Thermal Aging on Mechanical Damage/Failure of Alloy-22 Outer Barrier from Mechanical Means Such as Seismic Activity
	Uncertainty and Variability of the Effects of Material and Manufacturing Defects on the Corrosion Degradation Processes Above
Representation of Uncertainty and Variability of Waste Package and Drip Shield Degradation Processes in WAPDEG Analysis	Conceptual Model(s) for the Method and Approach to Represent Uncertainty and Variability of Exposure Conditions for Waste Package and Drip Shield Degradation in WAPDEG Analysis
	Conceptual Model(s) for the Method and Approach to Represent Uncertainty and Variability of Individual Degradation Processes of Waste Package and Drip Shield and Their Parameters in WAPDEG Analysis

The initial perforation is assumed to allow the initiation of waste form degradation inside the breached waste package. Likewise, if under dripping, the initial perforation of the drip shield is assumed to allow the initiation of dripping on the underlying waste package. The perforated area on the waste package is the effective area through which radionuclides will be transported and released. Under dripping condition, the perforated area on the drip shield provides the area through which seepage into the emplacement drift flows onto the underlying waste package.

Uncertainty and spatial variability of the degradation effects are also provided in the WAPDEG code output.

In general, waste package and drip shield degradation will be handled as realistically as possible in WAPDEG. However, where defensibly justified, WAPDEG will be simplified. The simplification may include the omission of some of the degradation modes. For instance, if corrosion of the inner barrier is found to be immaterial to performance, it might be omitted when WAPDEG is coupled to the TSPA model.

The major differences between the TSPA-SR and TSPA-VA planned in the area of waste package and drip shield degradation are as follows:

- The TSPA-SR models will address the new design, including drip shields, backfill, a waste package with the corrosion resistant material on the outside.
- The TSPA-SR models will consider additional corrosion mechanisms, such as SCC and long-term phase stability.
- For the TSPA-SR, the waste package and drip shield degradation model (WAPDEG) will be integrated with the TSPA model (RIP), thereby allowing time-dependent changes in the environment to be considered directly.

A more mechanistic approach to calculating the probability and consequences of manufacturing defects and other possible causes of premature failures may be included in TSPA-SR.

3.4.6 Sensitivity Analysis

A series of sensitivity analyses will be conducted on the waste package and drip shield performance in TSPA-SR to study the effects several important factors, possibly including the following:

- Key corrosion process parameters
- Alternative interpretations or uses of corrosion model and data in the model abstraction
- Major WAPDEG modeling assumptions
- Alternative waste package and EBS design options
- Alternative conceptual models in waste package and drip shield degradation analysis.

These analyses should provide greater insights into waste package and drip shield performance attributes, as well as better support for the technical basis of the waste package model for the TSPA-SR. The following highlights some of the key sensitivity analyses that are presently planned to be conducted (note that as the work for TSPA-SR progresses, not all of these analyses may prove to be necessary or appropriate).

Patch Size–A patch area on waste package and drip shield used in WAPDEG analysis is defined as the maximum area over which a uniform exposure condition is assumed and, thus, a uniform general corrosion rate is applied (Section 3.4.5). In the TSPA-SR analysis, the patch area for waste package and drip shield will be sampled randomly over a range to be defined later and based on relevant data and analysis. Effects of the patch size will be analyzed by assigning alternative distributions to the patch size. The alternative distribution parameters (i.e., distribution type, mean or median, standard deviation if applicable, minimum and maximum of distribution if applicable, and others) will be developed from relevant data and analysis.

Wetted Area By Drips–The wetted area on waste package and drip shield by drips is an uncertain parameter. It has a significant impact on the waste package and drip shield performance, because, in the current conceptual model in WAPDEG analysis, all the localized corrosion modes (pitting corrosion, crevice corrosion, SCC and HIC) for waste package and drip shield are only possible for those patches wetted by drips. This conceptual model is based on the rationale that, under the expected repository conditions, aggressive species (i.e., chloride ions that are required to initiate and sustain the localized corrosion processes) can be supplied to the corroding sites only by the groundwater seepage reaching the waste package and drip shield. In the TSPA-SR analysis, the wetted area for waste packages and drip shields under seepage will be sampled randomly over a range that will be defined later and based on relevant data and analysis. Effects of the wetted area will be analyzed by assigning alternative distributions to the patch size. The alternative distribution parameters, such as the distribution type (mean or median), standard deviation (if applicable), and minimum and maximum of the distribution (if applicable), will be developed from relevant data and analysis.

Water Chemistry on Waste Package and Drip Shield–The in-drift geochemistry model abstraction will represent the temporal evolution of water chemistry on the waste package and drip shield surfaces, with an appropriate range for the spatial variability. The abstraction will also provide uncertainty of the water chemistry evolution. Because of the complexity involved in the geochemistry in the perturbed near-field of the repository, the analyses results are expected to be uncertain. Effects of potential variations in the water chemistry evolution on waste package and drip shield surfaces will be analyzed with alternative interpretations to the TSPA-SR analyses results.

Cyclic Wet and Dry Conditions–Waste packages and drip shields that come in contact with seepage in the repository have a potential to experience cyclic wet and dry conditions. Such a cyclic condition is likely to generate highly concentrated salt solutions on the wetted area of the waste package and drip shield surfaces for extended time periods until the emplacement drift conditions become sufficiently wet (i.e., high relative humidity). These conditions, if they occur in the repository, are likely to provide the most favorable conditions for corrosion degradation. Effects of the cyclic wet and dry conditions will be studied by extending the time period for the most corrosive condition and by applying the corrosive condition to the initiation and propagation of corrosion degradation processes considered in the analysis.

Alternative Conceptual Models for SCC Initiation–If SCC of the waste package outer barrier (Alloy-22) is initiated, it would be the dominant degradation mode that could limit the service life of waste packages. The SCC initiation threshold is highly dependent on the material and the physical and chemical exposure conditions in which the material exists. There are several conceptual models for SCC within the corrosion science community. Some of the most widely accepted alternative conceptual models for SCC initiation will be employed in the analysis to investigate their effects on waste package performance and the TSPA.

Alternative Thresholds for Crevice Corrosion Initiation–The TSPA-SR analysis will use a critical crevice corrosion potential as the primary threshold parameter for crevice corrosion initiation of the waste package and drip shield. The potential will be expressed as a function of temperature and the chemistry of the contacting solution. Alternatively, as was used in the TSPA-VA analysis, a critical threshold temperature has also been used as an initiation threshold parameter for crevice corrosion, assuming aggressive water chemistry is inside the crevice. The critical temperature based approach is generally more conservative than the corrosion-potential-based approach. Sensitivity analysis will be conducted to study the effects of the alternative thresholds for crevice corrosion initiation. The critical threshold temperature will be developed from relevant data and analysis.

Effect of Microbial Activity–Although there have been no documented cases for the susceptibility of Alloy-22 and titanium-7 to microbiology influenced corrosion, microbiological processes, if they occur in sufficient numbers in a localized area, could raise the corrosion potential of the alloys. Thus, it would make them more susceptible to localized corrosion attack. Sensitivity analysis will be conducted to study the effects of microbial activity on degradation of the waste package and drip shield by elevating the corrosion potential. The corrosion potential elevation will be determined based on relevant data and analysis.

Material and Manufacturing Defects–In the TSPA-SR, manufacturing and materials defects in the Alloy-22 outer barrier and the titanium-7 drip shield are represented with the presence of flaws in the materials. The presence of such defects causes the materials to be more susceptible to localized corrosion (crevice corrosion, SCC, and HIC for drip shield) and enhances the propagation rate of those corrosion processes. The occurrence of undetected defects and their sizes in the Alloy-22 outer barrier and in the titanium-7 drip shield will be represented with probability distributions, and their effects are represented by coupling them with the localized corrosion processes. Sensitivity analysis will be conducted to study the effects of alternative interpretations of the material and manufacturing defects by assigning alternative distributions to the occurrences and sizes of defects.

Rockfall Effect–The EBS design includes backfill; therefore, potential rockfall damage to the waste package and drip shield is not a concern in the TSPA-SR analysis. Sensitivity analysis might be conducted to investigate the effect of rockfall damage to the waste package and drip shield for a no-backfill design option. As appropriate, the rockfall sensitivity analysis will be conducted by incorporating the following components into the WAPDEG analysis: (1) rockfall frequency and rock size from seismic activity and TM stress; (2) stress analysis of the drip shield and waste package using combinations of predetermined rock sizes and thicknesses of the drip shield and waste package, with the analysis results grouped into three categories no effects, generation of an incipient crack, or a through-wall crack; and (3) real time coupling of the analyses above, with corrosion degradation of the drip shield and waste package.

Additional sensitivity analyses are planned for alternative design options for the waste package, drip shield, and other EBS components, and for alternative representations of repository TH conceptual models such as climate change and percolation flux.

3.4.7 Treatment of Uncertainties

For the TSPA-SR, the process level models and abstraction account for uncertainty and variability in the waste package and drip shield component; however, there is a concern with the degree of uncertainty and variability for these components. If the uncertainty and variability associated with parameters and models describing waste package and drip shield lifetimes are overestimated, performance can be significantly overestimated because failures could be artificially spread out in time. For example, peak doses could be much lower if container failures span a 100,000-year time period rather than a 10,000-year period, which would be the case if uncertainty or variability are overestimated. Equally as important, if uncertainty and variability for a regulatory standard with a time limit are underestimated, then performance within the time limit can be significantly overestimated (e.g., if container failures all occur at 50,000 years, there will be no releases within the 10,000-year regulatory time limit). To a certain degree, the situation is similar to other TSPA components. But with the emphasis on a robust design, most waste packages and drip shields would not be expected to fail in the 10,000-year period. Thus, failures would only be calculated to occur (if at all) because of uncertain or varying conditions or degradation processes.

For the VA, an expert elicitation was held to determine corrosion rates for the waste package materials. No attempt was made to differentiate between uncertainty (the lack of knowledge concerning the exact corrosion initiation threshold and degradation rate of a material) and variability (the differing corrosion initiation thresholds and different degradation rates that could occur because of different or varying material properties (on a microstructural scale) and temporal or spatial exposure conditions). The elicited corrosion rates were defined with probability distributions, and these distributions were interpreted to represent the combination of both uncertainty and variability in a corrosion rate. For the TSPA-VA calculations involving WAPDEG, an attempt was made to separate the uncertainty and variability components of the distributions. The result was three container lifetime distributions representing uncertainty, with restricted variances representing the idea that the variability is only a portion of the variance ascribed to the initial distributions.

For TSPA-SR, the objective is to estimate degradation rates from data to the extent possible. Other uncertainty or variability problems are associated with this course of action. The materials planned for the construction of the drip shield and waste package (titanium-7 and Alloy-22, respectively) are relatively recent creations, and there are no natural analogs to investigate their degradation over long time periods. Data being taken on the longevity of these man-made materials are necessarily abbreviated, requiring extrapolation to long time periods. Further, because of the complexity of the possible waste packages and drip shields environment, it is impossible to test them all. Finally, the scale of corrosion on a waste package or drip shield is much smaller than the scale at which flow and chemistry are calculated.

Given this background, the strategy for dealing with uncertainty and variability in WAPDEG for TSPA-SR (as in all TSPAs) is to capture, somewhere in the results, the actual behavior of the system, and to err on the side of overestimating container degradation, if necessary. One possible approach is as follows. (Note that the discussion here is generalized to an idealized metric, a degradation rate. In actuality, parameters within the WAPDEG modules would have to be examined to determine how to best implement this method.) The following method should address the artificial improvement to performance that can be inadvertently gained by inappropriately including uncertainty; it also addresses variability.

Two distributions describing degradation rates can be specified for each degradation mode (1) a continuous distribution of the mean degradation rate, and (2) a continuous distribution of the standard deviation of the degradation rate. The first distribution is intended to represent the uncertainty in the average degradation rate. The second distribution is meant to represent the uncertainty in the variability of the degradation rate. The distribution of possible means must have an arbitrary component (i.e., the actual uncertainty in the degradation is probably greater than that which can be seen in the data, primarily because of the coarse resolution of the data and the necessity to extrapolate to long time periods). The distribution of possible standard deviations also must be somewhat arbitrary, although variability can be estimated from different rates seen in the data (i.e., the corrosion samples show different corrosion rates across their surface). Both distributions must take into account the differing seepage, chemical, and thermal environments in the repository, either with an increase in the variance or by developing different distributions for the different environments.

The WAPDEG code could be used to sample from these distributions to select the parameter values used in the calculation of the waste package and drip shield lifetime and degradation area distributions. In the TSPA-SR, the waste package and drip shield lifetime and degradation area distributions would be used in the calculation of water contact with the waste and subsequent radionuclide releases. It is anticipated that most waste package and drip shield failures would occur after the 10,000-year regulatory time frame. This method would allow an estimate of the probability of waste package and drip shield failure within the 10,000-year period. This estimate could be used to scale the results of a separate consequence analysis, or a screening could be made, either before or during the TSPA calculation, to restrict the TSPA calculation to only those situations where releases within 10,000 years are possible. Finally, a statistical sampling scheme could be devised where only those parameters that lead to releases would be sampled within the TSPA calculation. The results of these last two methods would have to be weighted by the probability of occurrence.

In the above scheme, the impetus is to allow the possibility of failures before 10,000 years, if allowed by our uncertainty in, and the variability of, the degradation processes. By structuring the uncertainty and variability distributions in this manner, the values of the distributions that fall farthest from the distribution medians (i.e., the tails of the distributions) might produce this behavior. There is an inherent inaccuracy when attempting to sample the tails of distributions that were defined with an arbitrary component. This method would not necessarily achieve the best estimate of waste package and drip shield performance within 10,000 years. The main benefit of using this method is that sensitivity analyses and regression analyses could be used to allow an understanding of what is important in this area, and what (or whether) additional information is needed to address uncertainty and variability in the waste package and drip shield component.

3.5 WASTE FORM DEGRADATION MODEL

3.5.1 Introduction

The purpose of the waste form degradation model is to evaluate the rate of degradation of cladding and the waste matrix, the rate of mobilization of radioisotopes, and the migration of radioisotopes through remaining portions of the waste package.

3.5.2 General Description of Process Models and Abstraction

The primary features and processes in the model of the degradation of the waste form discussed in this section include the following:

1. Grouping of the various waste forms and the corresponding radioisotope inventory
2. Degradation of Zircaloy cladding on CSNF

3. Alteration rate of waste form matrix
4. Concentration limits on radioisotopes
5. Formation of colloids
6. Advection and diffusion of radioisotopes through the alteration products into the drift.

The coupling of these features and processes is illustrated by the flow diagram in Figure 3.5-1.

3.5.2.1 Waste Form Categories

Four major categories of waste forms potentially would be included in the Yucca Mountain repository:

1. CSNF. 62,968 metric tons of heavy metal (MTHM)—irradiated uranium dioxide pellets encased in cladding from commercial power reactors

2. DSNF. 2,333 MTHM—miscellaneous SNF including 65 MTHM of naval fuel, but primarily consisting of irradiated uranium metal encased in cladding used in the production of plutonium (N-Reactor)

3. HLW. 4,667 MTHM—radioactive waste from reprocessing either CSNF (640 MTHM) or DSNF (4,027 MTHM) that is in solid solution with borosilicate glass

4. Plutonium waste (50 MTHM). Mixed-oxide SNF (32 MTHM) and plutonium waste in solid solution with glass ceramic (18 MTHM).

This totals slightly over the 70,000 MTHM legal mass capacity of the repository, but would be adjusted at time of emplacement. Of the 70,000 MTHM, 63,000 MTHM (90 percent) is allocated for CSNF and 32 MTHM for the mixed-oxide. The remaining 7,000 MTHM (10 percent) is allocated to the second and third categories and about 18 MTHM to the fourth category.

3.5.2.1.1 Commercial Spent Nuclear Fuel

The CSNF consists of two categories based on the type of nuclear reactor for which it was designed; fuel from pressurized water reactors (PWR) and fuel from boiling water reactors (BWR). The size of the fuel rods and assemblies of fuel rods differ, therefore the amount of decay heat produced in a disposal container holding PWR or BWR SNF also differs. Most of the fuel within these two categories is clad with Zircaloy; however, about 700 MTHM (~1 percent of the repository mass capacity) is old fuel that is clad with stainless steel. The age of the fuel varies from the minimum allowed age (5 years) to a little over 50 years. Past TSPAs have used an estimate of the radioisotope inventory that was produced in the early 1990s, but the TSPA-SR will use an updated radioisotope inventory.

3.5.2.1.2 U.S. Department of Energy-Owned Spent Nuclear Fuel

The DSNF consists of more than 250 distinct types of spent fuel with a combined mass of about 2,500 MTHM. These types of fuel can be grouped into 11 categories (e.g., naval SNF represents about 3 percent of the combined heavy metal mass MTHM). However, one fuel type, the uranium metal, N-Reactor fuel stored at Hanford, represents about 90 percent of the combined mass (Rechard 1998, p. 11-2; CRWMS M&O 1998a, Chapter 6, Table 6-5). Although the N-Reactor fuel is Zircaloy-clad, the cladding will not be included in performance calculations because it generally is in poor condition. Rather, the TSPA-SR will use only the degradation behavior of N-Reactor fuel matrix to conservatively represent the DSNF category. The weighted average of all fuel types (except naval SNF) will be used for the inventory. The Assistant Secretary of Environmental Management of DOE/Environmental Management will provide a slightly revised inventory for the TSPA-SR. Also, the TSPA-SR will use the degradation behavior of the Zircaloy-clad CSNF to conservatively bound the behavior of the naval SNF.

3.5.2.1.3 High-Level Radioactive Waste

The HLW in solid solution with borosilicate glass has been, and continues to be, produced at Savannah River Site. In addition, a small amount was produced at West Valley Demonstration Project in New York. HLW eventually will be produced and stored at two other sites—Hanford Reservation and Idaho National Engineering and Environmental Laboratory (INEEL). Depending on the schedule for the completion of the potential YMP repository and construction of the waste processing facilities at each site, both could send HLW to the repository. Because the SNF that was processed at various sites differed, the radioisotope inventory of the HLW will vary slightly among the sites. But, as for past TSPAs, an average inventory will be used for TSPA-SR. However, the average will be reevaluated for TSPA-SR.

3.5.2.1.4 Plutonium Waste

The U.S. expects to reduce its stockpile of excess weapons grade plutonium by converting it to a mixed-oxide fuel for use in commercial reactors or by direct disposal of plutonium in glass ceramic. The direct disposal and mixed-oxide fuel waste is planned for disposal in the potential repository at Yucca Mountain. However, the amount is so small that the inventory for this waste category for the TSPA-SR will be included in the respective inventories of HLW and CSNF.

3.5.2.2 Radioisotopes Important to Total Systems Performance Assessment–Site Recommendation

Over 100 radioisotopes are present in the waste forms to be disposed of at the potential Yucca Mountain repository. However, only a limited subset is potentially important to either heat production or hypothetical doses to humans.

Eight radioisotopes will be used to evaluate heat production from the waste. The most important isotopes are cesium-137 and strontium-90 and their respective daughters, barium-137 m and yttrium-90 (in secular equilibrium). Radioisotopes of secondary importance for heat production are plutonium-238, plutonium-240, americium-241, and curium-244.

The TSPA-VA tracked the migration of, and dose from, nine radioisotopes (technetium-99, iodine-129, neptunium-237, uranium-234, plutonium-239, plutonium-242, selenium-79, protactinium-231 (assumed in secular equilibrium with uranium-235), and carbon-14). This list will be reevaluated for the TSPA-SR because early performance assessments used an informal screening that was based on the now obsolete 40 CFR 191 EPA Standard. Elements that may be added include actinium, radium, thorium, and americium. However, other elements also will be evaluated to ensure that the radioisotopes transported represent 99 percent of the potential dose received by humans.

3.5.2.3 Degradation of Commercial Spent Nuclear Fuel Cladding

Since the 1950s, most CSNF has been clad with less than 1 mm (usually between 600 through 900 μm) of Zircaloy, an alloy that is about 98 percent zirconium with small amounts of tin, iron, niobium, and chromium. Zircaloy is very resistant to corrosion and, on average, cladding failure is expected to be minimal (less than 5 percent) in the first 10,000 through 100,000 years. However, because Zircaloy provides such excellent protective properties on average, characterization of the uncertainty in its performance is important.

3.5.2.3.1 Modes for Initial Cladding Breach

Initial breach of the cladding may occur because (1) the cladding initially fails within the reactor or during storage, (2) debris falling from the roof of the tunnel physically crushes or otherwise penetrates the cladding, or (3) the cladding fails from localized corrosion. In TSPA-VA, the failure of PWR cladding was assumed to bound the failure of BWR cladding because the PWR cladding is typically thinner than BWR cladding. For PWR cladding, the initial cladding failure percentage was set at 1.25 percent, the majority of which (1.15 percent) was stainless steel cladding. PWR cladding failure from debris was assumed to begin after the disposal container had sufficiently weakened (in all cases, 10^5 years after initial penetration of the disposal container) and then increase linearly on a log scale thereafter from 0.2 percent at 10^5 years after initial penetration to a sampled value at 10^6 years after initial penetration that varied between 0.2 percent and 11 percent. PWR cladding failure from localized corrosion was evaluated using WAPDEG, with a localized corrosion rate 10 to 1,000 times smaller than Alloy-22. Using these assumptions, the amount of fuel exposed at 10^6 years varied between 0.3 and 40 percent (mean of 7.8 percent). For TSPA-SR, mechanisms of localized failure (such as delayed hydride cracking) will be reevaluated.

In TSPA-VA, the non-Zircaloy-clad (mostly stainless steel cladding) fuel was distributed homogeneously throughout the repository. For the SR repository design, this fuel will be consolidated into separate waste packages that would have much higher initial failure of cladding, while the vast majority of the waste packages (those with Zircaloy-clad rods) will have much lower initial failure.

3.5.2.3.2 Modes for Increasing Cladding Failure after Breach

After the cladding has initially been breached, the clad may unzip because the fuel volume increases during oxidation of the UO_2 (Section 3.5.2.4), (i.e., the replacement of the initial UO_2 with more oxidized phases causes enough pressure by volume expansion to burst the cladding from within). The viability of this mechanism for increasing the exposed surface area of the matrix is sensitive to environmental conditions such as temperature, which is discussed below. In the TSPA-VA, the temperature of the cladding and matrix was not high enough nor did it occur for a long enough period to cause unzipping in a dry environment, and so the phenomenon was not included. Although the work will be reevaluated for the TSPA-SR, conditions for unzipping in a dry environment probably will be unlikely. Conditions for unzipping in a wet environment is more likely; therefore, the TSPA-SR also will evaluate the possibility of the clad unzipping in a wet environment.

3.5.2.3.3 Temperature History of Cladding

Evaluation of the modes of localized corrosion requires an estimate of cladding temperature. The TSPA-SR will evaluate a defensible functional relationship of the difference of average surface temperature of the disposal package and the temperature of the cladding, based on a heat conduction model.

3.5.2.4 Degradation of Commercial Spent Nuclear Fuel Waste Matrix

Under oxidizing conditions in the presence of liquid or vapor water, the UO_2 in CSNF is not stable and alters to the +6 valence in the uranyl molecule, UO_2^{2+} which is far more mobile; thus, the alteration rate can potentially effect the release of radioisotopes. The conceptual model, the TSPA-SR abstraction and corresponding assumptions, and any uncertainty of the model parameters for the alteration of the CSNF matrix are discussed below.

3.5.2.4.1 Kinetic Rate Equation for Wet and Humid Conditions

In the TSPA-VA, the alteration rate of UO_2 is fast (~1,000 years) relative to the regulatory period; therefore, the release rate of moderately soluble radioisotopes such as neptunium-237 was not controlled by the rapid alteration rate of the CSNF matrix. Only release rates of highly soluble radioisotopes such as iodine-129 or technetium-99 were influenced by the alteration rate of the CSNF matrix. For the TSPA-SR, the rate at which the CSNF waste matrix degrades under humid or wet conditions will be expressed as a classic chemical kinetic equation, where the terms of the coefficients of the equation have been evaluated through regression analysis on experimental data obtained over a range of temperatures, water chemistry (total carbonate concentration, and pH), and oxygen concentration (CRWMS M&O 1998a, Chapter 6, p. 6-62).

Because it is important to provide a general qualitative description of the degradation mechanisms involved and how they are influenced by solution chemistry (Eh, pH,) as the CSNF alters, the performance assessment models will qualitatively relate the various phenomena to the empirical terms to demonstrate the reasonableness of the model.

3.5.2.4.2 Experimental Data Available

Degradation of the CSNF can occur under a wide range of environmental conditions including wet or dry, anoxic or oxic, high or low temperature, high or low total carbonate concentration, high or low pH, and high or low fuel burnup. The YMP has spent several years collecting data on the dissolution of UO_2 in the CSNF under conditions applicable to the potential Yucca Mountain repository.

3.5.2.4.3 Inventory of Radioisotopes Readily Released

A small percentage of the inventory of volatile radioisotopes (i.e., technetium-99, iodine-129, cesium-135, cesium-137, selenium-79, and carbon-14) resides in the gap between the fuel pellets and the CSNF cladding. This gap inventory can be released immediately once the cladding is breached. Since TSPA-1995 (CRWMS M&O 1995), the YMP has assumed that (except for carbon-14) 2 percent of the inventory of the volatile radioisotopes resides in the gap. For carbon-14, the analysis has used a uniform distribution between 1.25 percent and 5.75 percent since TSPA-1993 (CRWMS M&O 1994; 1998a, Chapter 6, Table 6-27). The TSPA-SR will reevaluate these percentages based on the most current data.

3.5.2.4.4 Corresponding Effective Surface Area

The effective surface area of the CSNF is the constant specific surface area (m^2/g) times the mass that is exposed as the cladding fails. In the TSPA-SR, as in TSPA-VA, the mass used to compute the effective surface area will be proportional to the surface area of failed cladding. In the TSPA-SR, a surface area of CSNF will be evaluated that is consistent with the assumptions of the degradation rate equation and clad unzipping equation.

3.5.2.5 Degradation of U.S. Department of Energy-Owned Spent Nuclear Fuel Waste Matrix

The degradation behavior of DSNF (except the naval SNF) will be represented by the metallic uranium SNF from N-Reactor. For TSPA-VA, the model for the degradation of metallic uranium was a classic Arrhenius kinetic rate equation using parameters from assessments of SNF and HLW (Rechard 1995, p. 11-22; 1998, p. 7-32; see also CRWMS M&O 1998a, Chapter 6, p. 6-69). The overall degradation rate was the Arrhenius rate times the effective surface area. In TSPA-VA, the effective surface area was five times the geometric surface area. Because the degradation rate estimate by the Arrhenius equation was so rapid, the sensitivity of the results to varying the multiplier for the geometric surface area between 0.1 and 100 (and thus the overall degradation rate) was small. Nonetheless, there was little applicable experimental data to substantiate the parameter values selected. TSPA-SR will use a degradation rate and a corresponding effective surface area that bounds the experimental data on N-Reactor fuel collected over a range of conditions in the last few years.

3.5.2.6 Degradation of High-Level Waste Matrix

3.5.2.6.1 Aqueous Degradation Model

Glass is a thermodynamically metastable, covalent/ionic solid whose degradation depends on ion exchange, surface complexation, and silica concentration. These three processes, in turn, depend upon temperature. The model to be developed for aqueous degradation of HLW in TSPA-SR will be similar to that in TSPA-VA where silica concentration and temperature were the primary variables (CRWMS M&O 1998a, Chapter 6, p. 6-73):

$$r = k_{short}\,(1 - [SiO_2]/a) + k_{long} \qquad \text{(Eq 3.5-2)}$$

where

k_{short} = short-term rate parameter dependent on temperature and pH

$[SiO_2]/a$ = saturation index, where $[SiO_2]$ is concentration of dissolved silica and a is silica concentration at saturation and dependent on glass composition

k_{long} = long-term rate parameter, dependent on temperature, once solution is fully saturated with silica

The rate parameters are determined by a linear regression fit to experimental data over a range of temperature (and pH for k_{short}) from flow through experiments. TSPA-SR will update the rate parameters using additional experimental data.

3.5.2.6.2 Vapor Hydration Model

When a disposal container breaches, water vapor may be the first reactant to enter the container. In TSPA-VA, a separate alteration model for vapor hydration of the HLW glass was not used; however, water vapor could alter the glass to produce a gel layer containing high concentrations of radioisotopes. This altered glass would then have a higher release rate than unaltered glass, after liquid water entered the breached disposal container. TSPA-SR will evaluate the sensitivity to this sequence of events by developing a vapor hydration model for the borosilicate glass.

3.5.2.6.3 Corresponding Effective Surface Area

In TSPA-VA, the effective surface area of HLW was set at 21 times the geometric surface area (CRWMS M&O 1998a, Chapter 6, p. 6-79). This multiplication factor will be reevaluated for TSPA-SR.

3.5.2.7 Concentration Limits

As in previous TSPAs, the mass of radioisotopes released (based on the degradation rates of the CSNF, DSNF, or HLW matrix) will be compared to the maximum dissolved mass possible (based on water flowing through the disposal container and specified concentration limits). If the maximum dissolved mass is less than the mass of radioisotopes liberated from the waste matrix, the mass will be set to the dissolved mass and the difference will be assumed to precipitate out of solution and be available for transport at later times. The concentration limit usually is the solubility limit of pure phase species of the various radioelements, as discussed in the next section. However, experiments have shown much lower concentrations in solution for some critical radioisotopes such as neptunium-237. As mechanistic base models are developed and experimentally confirmed, the pure phase range may be extended to lower values to include mixed phase effects.

3.5.2.7.1 Pure Phase Solubility Limits

Usually, the concentration limits for each radioisotope transported in the TSPA-SR will be expressed as a distribution of values. However, the concentration limit for uranium and neptunium, for which sufficient data are available, will probably be expressed as a function dependent on water chemistry (pH, Eh, and $[CO_3]_T$). Under equilibrium conditions, the concentrations of radioisotopes in solution are limited by the solubility products of the solid phases that contain the radioisotopes (either solid phases with the radioisotope as the dominant element or solid phases with trace amounts as can occur with coprecipitation). The solid phases that form depend on the temperature, redox conditions, and species in solution in the groundwater. Uncertainty in the precise values for these variables in the waste package and emplacement drifts results in a wide distribution of possible concentration limits. For TSPA-VA, the distribution of each radioisotope transported was primarily based on an elicitation of experts both inside and outside the YMP, conducted in 1993 (Wilson et al. 1994, pp. 9-1 through 9-11; CRWMS M&O 1998a, Chapter 6, Table 6-32).

For TSPA-SR, a reevaluation of radioisotope solubility is planned. A distribution of concentration limits for important radioisotopes will first be based on a wide variety of chemical conditions. Although scientific judgment will be necessary to define the solid phases present and range of water chemistry, determination of the range of the distribution will be facilitated by using EQ3NR, a chemical equilibrium code, based on either thermodynamic data available from respected sources, such as the database maintained by the NEA of the Organization for Economic Cooperation and Development, or review of literature data (CRWMS M&O 1998a, Chapter 6, p. 6-95). The distribution will later be refined and narrowed as information becomes available on the design of the engineered barrier, fluid flow rates, and thermal history.

3.5.2.7.2 Sensitivity Cases

One potential alternative model parameter distribution is possible based on mixed phase concentration limits. Experiments with SNF show neptunium-237 concentrations much lower than would be predicted through pure phase equilibrium. Therefore, the lower range of the solubility limit for neptunium may be revised to incorporate this observation if the experimental evidence is sufficiently defensible. One possibility is that NpO_2 is the solid phase controlling the concentration as suggested by experiments. Another possibility is that an important mixed phase or sorption mechanism is controlling the concentration of neptunium-237 in solution. For example, in the past two years, some experimental evidence was collected suggesting that neptunium-237 is encapsulated in the secondary phases of uranium as the initial UO_2 degrades (specifically, in a uranyl hydroxide mineral, schoepite) (CRWMS M&O 1998a, Chapter 6, p. 6-118). However, in contrast to this evidence, uranyl silicates such as Na-boltwoodite also form without showing evidence of encapsulating neptunium. This conflicting evidence might occur because the amount of neptunium-237 originally in the SNF is small and difficult to locate, or because of differences in charge balancing for the two mineral species.

3.5.2.8 Formation of Colloids

Particles between 1 nm and 1μm are small enough to be easily suspended and transported in liquid, and are generically described as colloids. When a radioisotope is solubility limited, releases may be further increased if the radioisotope tends to form colloids directly or has an affinity for any mobile colloids present in the mobile liquid. Furthermore, the transport velocity may be faster than those of dissolved radioisotopes that sorb onto the surrounding rock (if the radioisotopes do not readily (reversibly) detach from the colloids).

3.5.2.8.1 Radioisotopes Susceptible to Colloidal Transport

Radioisotopes that have low solubility and high sorption onto components of the engineered barrier or geologic barrier are likely to have the largest percentage changes in releases when colloidal transport is considered. Of these radioisotopes, only those that are a major part of the waste inventory and have potentially large dose conversion factors are of potential importance to the performance of the disposal system. Plutonium meets these screening criteria and was considered in TSPA-VA (CRWMS M&O 1998a, Chapter 6, p. 6-97). In addition to plutonium, other radionuclides, such as americium and cesium, will be considered for TSPA-SR.

3.5.2.8.2 Colloid Formation

Natural colloids potentially present in the repository include those already present in the geosphere such as microbes, organics (humic and fluvic acids), and mineral colloids (such as goethite, hematite, and clay, primarily smectite). Colloids that will be present in the repository also include those produced from degradation of the disposal package (mineral colloids) and degradation of the waste matrix (e.g., clay particles from borosilicate glass and spallation from CSNF and DSNF). Those colloids assumed to be present in sufficient quantities to affect repository performance will be naturally occurring clay, naturally occurring silica, iron corrosion products (goethite and hematite), SNF matrix products, and HLW matrix products. As in TSPA-VA, the actual concentration of colloids (C_C) will be evaluated from a linear empirical relation with ionic strength of the liquid solution. However, additional data will be added for the TSPA-SR analyses that were not used for TSPA-VA.

3.5.2.8.3 Reversibly Sorbed Colloids

Radioisotope attachment to colloids will be modeled using two extremes (1) instantaneously reversible attachment, and (2) totally irreversible attachment. The colloid concentration with reversibly attached radioisotopes (C_R) will be defined assuming equilibrium through an effective partition coefficient (K_d) (i.e., $C_R = K_d(m)\ C_C$) where the partition coefficient is a function of the type of colloid (m) (either clay, silica, iron corrosion product, CSNF, or DSNF colloid). As in TSPA-VA (CRWMS M&O 1998a, Chapter 6, p. 6-100), $K_d(m)$ for clay, silica, and iron corrosion products will be evaluated from sorption/desorption experiments of Pu(IV) and Pu(V) (Liu et al. 1998). $K_d(m)$ for SNF and HLW will again be evaluated based on observed colloids formed during the unsaturated drip tests (Finn et al. 1997). However, for both minerals and SNF, some new data are available and will be used for TSPA-SR. Furthermore, sorption/desorption experiments will be done on the colloids obtained from degradation of HLW.

3.5.2.8.4 Irreversibly Sorbed Fraction of Colloids

As in the TSPA-VA, the division between reversibly and irreversibly sorbed radioisotopes on colloids will be sampled. Furthermore, the irreversibly sorbed fraction will be treated as a nonsorbing contaminant with a small diffusion coefficient.

In the TSPA-VA, the parameter distribution for the fraction of radioisotopes irreversibly sorbed on colloids was estimated using preliminary information from the Benham nuclear test area at the NTS. The Benham data showed rapid transport of colloid associated plutonium occurred (Thompson 1998, p. 13, 18). To better substantiate this information, however, the TSPA-SR will instead use experimentally observed desorption rates (Liu et al. 1998) to estimate the irreversibly sorbed fraction. The estimated irreversibly sorbed fraction from these experiments will likely be much larger than those estimated from the NTS, because the tests have been run for such a short time and should provide a conservative upper bound for the distribution. This higher fraction of irreversibly sorbed colloids may make plutonium more important to dose relative to technetium.

3.5.2.9 In-Package Transport

TSPA-SR will most likely neglect any transport resistance in the waste package (e.g., it is unlikely that credit will be taken for sorption on corrosion products). However, if a large effect on performance is apparent (e.g., from a bathtub scenario) then a simple model of transport within the package may be appropriate.

3.5.3 Summary of Key Waste Form Assumptions

The waste form section has been formatted differently from other subsections of Section 3, due to its many diverse topics. For the ease of the reader, the waste form assumptions are collected here, though they are pointed out within the text of Section 3.5.2. The assumptions are listed by topic.

- **DSNF**
  - Assume no credit for N-reactor cladding.
  - Use weighted average for the inventory of the 11 DSNF fuel types.
  - Use degradation behavior of zircalory-clad CSNF to model behavior of naval SNF.
  - Use degradation behavior of N-reactor fuel for all DSNF except naval fuel.
- **HLW**
  - Use average HLW inventory (not site specific).
  - HLW degradation model is a curve-fit to data.
- **Plutonium Waste**
  - Include Pu-waste in respective HLW and CSNF inventories.
- **Stainless Steel Cladding**
  - Assume Stainless Steel clad fuel is consolidated within a few waste packages, not spread homogeneously in all waste packages.
- **Cladding**
  - Assume heat conduction model to determine temperature of cladding relative to temperature of waste package surface.

- **CSNF Degradation**
  - CSNF degradation model is a curve-fit to data.
- **Colloids**
  - Major radioisotopes susceptible to colloidal transport are plutonium, americium, and cesium.
  - Colloids assumed to be present in sufficient quantities to affect repository performance are: naturally occurring clay, naturally occurring silica, iron corrosion products, SNF matrix products, and HLW matrix products.
  - Radionuclide attachment to colloids assumed to be either instantaneously reversible, or totally irreversible.
  - Treat irreversibly sorbed fraction as a nonsorbing contaminant with a small diffusion coefficient.
  - Use experimentally observed desorption rates to estimate irreversibly sorbed fraction.
- **In Package Transport**
  - Neglect in-package resistance to transport.

3.6 ENGINEERED BARRIER SYSTEM TRANSPORT

The EBS is comprised of all the components contained within the emplacement drift, including the drip shield and waste package (see Figure 3.3-1 for a depiction of EBS components in an emplacement drift). The transport of radionuclides within the EBS is determined by drip shield and waste package degradation, cladding and waste form degradation, TH and chemical environments, and the design of the EBS. Radionuclides released from the EBS enter the surrounding host rock where they become available for transport through the UZ.

The EBS transport process and abstraction models, major assumptions on which these models are based, and significant couplings between these models and other TSPA models are described in this section. In addition, sensitivity analyses to be performed and the treatment of important uncertainties in conceptual models and data are described in this section.

3.6.1 Introduction

The release of radionuclides into the natural environment is controlled by the transport of radionuclides out of the waste packages and through the invert. Key factors affecting the transport of radionuclides through the EBS are:

- Performance of the drip shield
- Performance of the waste package
- Protection provided by cladding

- Waste form degradation rate
- Entry and movement of water through a waste package
- Solubilities (dissolved concentration limits) of radionuclides
- Transport of radionuclides through and out of the waste package
- Transport of radionuclides through the invert below the waste package
- Colloidal transport of radionuclides.

The current repository design concept (CRWMS M&O 1999a) calls for cylindrical waste packages (see Section 3.4) to be placed in the emplacement drifts. This design concept also utilizes a drip shield and backfill to provide for defense-in-depth against the release of radionuclides, and it is further characterized by the use of steel ground support. Each waste package will be comprised of a 2 cm Alloy-22 CRM outer layer, a 5 cm stainless steel 316NG CAM inner layer, and various handling and spacing materials holding waste forms in place (i.e., waste package internals).

After emplacement of the waste packages, radioactive decay of the waste will heat the drifts and locally perturb the normal percolation of water through the mountain. As the drifts cool, some of the ground water percolating through the mountain may drip into the drifts and subsequently contact some of the drip shields. Through time, the drip shield, waste package, and other components of the EBS are expected to degrade. The metallic materials of the drip shield, waste package, and ground support are expected to undergo humid and wet corrosion. Under wet conditions, the metallic materials may undergo localized or generalized corrosion, which may result in breaches of the drip shields and waste packages.

Once a drip shield is breached, water may contact the waste package and initiate aqueous corrosion. Once a waste package is breached, water may enter the package as water vapor or as drips. If the cladding is also breached, radionuclides may start to dissolve in the water. The dissolved concentration of each radionuclide mobilized from the waste form cannot exceed the radionuclide solubility limit, unless suspended colloids are included. Colloids may be important for two reasons (1) they may increase the release of radionuclides from the waste package, and (2) they may increase the transport velocity of radionuclides. Radionuclides mobilized in water as dissolved or colloidal species may then be transported by advective and diffusive transport from the waste form, through the waste package, and out of breaches in the waste packages. Once outside the package, the radionuclides will be transported through the invert predominantly by diffusion (if water is not flowing through the invert) or by advection (if an appreciable amount of water is flowing through the invert).

3.6.2 General Description of Process Model and Abstractions

The radionuclide transport process model will include one-dimensional advective and diffusive transport, as well as retardation due to sorption and precipitation. This model will be input directly into the TSPA model RIP and will make use of the compartment or cell modeling capability within RIP. The radionuclide transport pathway from the waste form, downward to the edge of the EBS (i.e., the interface between the drift wall and the UZ) beneath the waste packages, will be defined, using the following RIP cells arranged vertically in the following order:

- A waste form and waste package cell that represents the release of radionuclides from the waste form and the transport of radionuclides in the waste package
- A degraded waste package cell that represents transport through corrosion products of the drip shield, waste package internals, and waste package pedestal
- Three cells that represent transport through the granular invert.

All of these cells require definition of volume, material properties, retardation properties, and radionuclide solubility limits. Both advective and diffusive transport mechanisms between cells will be accounted for by defining transport connections between cells. These connections require definition of diffusive release area between cells. A conservative assumption of no sorption is applied to the first waste form and waste package cell connection.

To develop conceptual process inputs for the EBS radionuclide transport model, several supporting subsystem model analysis activities will be conducted in the following areas:

1. In-drift water distribution and removal analyses. These analyses will attempt to quantify water seepage throughout the drift and will be abstracted and used as input to determine water flow through breached drip shields and waste packages and also in the RIP EBS radionuclide transport model to calculate advective radionuclide transport through the invert.
2. Analysis of water seepage through a breached drip shield. This information will be abstracted and used within RIP to calculate the amount of water contacting the waste package.
3. Water seepage into, through, and out of a breached waste package, including assessment of waste form surface area contacted by water.
4. Assessment of in-package evaporation potential due to thermal decay. This information will be used to determine if and when liquid water will be present in the waste package and available to facilitate radionuclide transport.
5. Assessment of the degradation and collapse of waste package inner structure (basket). This information will be used as input to in-package flow and sorption modeling.
6. Assessment of the potential for sorption of radionuclides on corrosion products of the waste package and waste package internals.
7. Colloidal radionuclide transport through the EBS components. This information will be used in combination with the transport of dissolved radionuclides to describe the release of radionuclides from the EBS to the UZ.

While many radionuclides have the potential for colloidal transport, the colloid analysis activity for the EBS will focus primarily on plutonium. Plutonium is a major part of the waste inventory and is the most likely radionuclide to be affected by colloidal transport. The attachment of plutonium to colloids will be modeled using two approaches (1) instantaneous reversible attachment, and (2) totally irreversible attachment. Partitioning of plutonium between these two categories will be treated as an uncertain parameter. As more data are obtained, the colloidal transport model may be refined to include additional radionuclides (i.e., americium; see Section 3.5.8) and sorption and transport mechanisms, such as filtration.

There are several inputs to the EBS radionuclide transport model, including:

- The release rate of radionuclides from the waste form
- The flux and chemistry of water moving through the waste package and invert (see (1), (2), and (3) above, and Section 3.3)
- The sorption properties of the EBS materials (e.g., waste package, corrosion products, invert materials)

The output from the EBS transport model will be a time rate of release of dissolved and colloidal radionuclides from the EBS into the UZ. Dissolved radionuclide concentrations mobilized from the waste form will then be constrained by the solubility limit of each radionuclide (Section 3.5). In some cases, the solubility constraints will be described as a function of water composition. Along the transport pathway in the EBS (i.e., from the waste form to the interface of the drift wall and UZ), the radionuclide concentrations will be checked against the solubility limit.

3.6.3 Significant Coupling with Other Models

The EBS transport model has connections with several EBS subsystem models, which are discussed below.

Water Distribution and Removal Abstraction–This model provides the water flux at various locations in the drift, such as through a degraded drip shield, around the drip shield, through a degraded waste package, around the waste package, and through the invert. Water flux through the package and through the invert is used to calculate radionuclide transport.

In-Drift Geochemical Environment Abstraction Model–This model provides the chemical conditions in the waste package and along the transport pathway from the waste package to the interface of the drift wall and UZ. Chemical conditions important to transport potentially include pH, total carbonate concentration, and precipitation/dissolution reactions that may alter the flow and transport properties of the invert.

Waste Package Degradation Abstraction Model–This model provides the waste package breached area (i.e., crevices, patches, and pits) as a function of time, which allows for advective and diffusive transport out of the waste package.

Waste Form Degradation–This model provides the time-dependent release of radionuclides available for transport out of the waste package because of waste form degradation.

Unsaturated Zone Transport–The EBS transport model provides the source of radionuclides to the UZ transport model component.

3.6.4 Major Assumptions

The overall 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 conditions:

- One-dimensional advective and diffusive transport processes, with solubility limited concentrations and linear sorption.
- One-dimensional water flow through a breached waste package, corrosion products, and invert.
- Radionuclide sorption onto corrosion products may be represented using linear K_ds.
- Colloids with potential effect on repository performance may be represented by the following types clay, silica, iron corrosion products, spent fuel matrix products, and glass waste matrix products.
- Actinide attachment to colloids may be modeled using a combination of two approaches instantaneous reversible attachment and totally irreversible attachment.

3.6.5 Implementation in Total System Performance Assessment–Site Recommendation

The EBS transport model will be developed within the TSPA model using the RIP compartment model capability. As defined in Section 3.6.1, the EBS will be discretized into several RIP cells. This discretization will allow geochemical differences among 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.

Implementation of the TSPA-SR EBS Transport model will include the following aspects:

- The in-drift water flow abstraction will define the amount of flow at a number of locations in the drift, including within the backfill, through the drip shield, the waste package, and the invert.
- In-package evaporation will be considered. Liquid water may not form in the waste package for several thousand years because of heat generation and evaporation. Advective and diffusive releases cannot occur until liquid water can form. This effect may be important for calculating release from defective waste packages (juvenile failures).
- Sorption of radionuclides on corrosion products of the ground support system, drip shield, waste package, internal waste package structures, waste package supports, the rail system, and possibly the invert materials, will be considered.

- The invert will be comprised of a granular material that may act as a diffusive barrier.

- The bottom boundary condition for the RIP implementation of the transport model will be set to zero radionuclide concentration in the host rock rather than at the drift wall. The location of this specified zero concentration will coincide with the point where UZ flow around the drift converges underneath the drift.

- The colloidal transport model may include additional radionuclides, such as americium (Section 3.5.8), and the additional transport mechanism of filtration, but these refinements are not expected in TSPA-SR, Revision 00.

3.6.6 Sensitivity Cases

A series of sensitivity cases for EBS transport will be conducted for TSPA-SR to determine which parameters strongly influence radionuclide release from the EBS. The following are key sensitivity analysis cases to be considered.

Diffusion Coefficient and Liquid Saturation in the Invert–Diffusion of radionuclides through the invert will be evaluated in modeling and sensitivity analyses. These analyses will evaluate the sensitivity of diffusive transport through the invert to different invert diffusion coefficient values. The range of values will be based on a literature survey of material properties, as well as experimental and test data.

Liquid Saturation and Water Flow in Engineered Barrier System Components–Liquid saturation and water flow have a significant effect on the release from the EBS attributable to diffusive and advective transport. Sensitivity cases will be conducted for various values of seepage into the drift.

Water Contact with Waste Form–The waste form degradation and radionuclide transport rates out of the waste package may be strongly influenced by the contact area between flowing water and waste form. A series of sensitivity analyses will be conducted for a range of contact areas between water and waste form to assess the effect of this parameter on radionuclide releases from the waste package and EBS. Part of this range of water contact areas could include the so-called bathtub scenario, wherein the waste package has breached at the top but not at the bottom, allowing water to fill the package to a certain height, which in turn causes total immersion of the fuel rods in the liquid phase.

Engineered Barrier System Material Sorption Properties–Sorptive properties (various types of adsorption and desorption) of radionuclides on the degraded EBS materials, inside and around the waste package, could have a significant impact on the transport behavior of the radionuclides. There are several types of well-known isotherms to describe adsorption behaviors of adsorbate, which are dependent 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.

The above sensitivity analyses will determine how important these parameters are to total system performance. Parameters that have a measurable influence on dose rate will be included as probability distributions over the range of their uncertainty. Those that have little or no influence on performance will be set at conservative bounding values, such as zero sorption, and 100 percent water contact.

3.6.7 Treatment of Uncertainties

Radionuclide release from the EBS to the UZ depends on:

- The amount of water flowing through the waste package
- The amount of water flowing through the invert beneath the waste package
- The radionuclide sorption behavior of corrosion products from the ground support system, drip shield, waste package, internal waste package structures, waste package supports, rail system, and possibly, the invert materials
- The mass of the various radionuclides in the flowing water.

Each of these quantities have a degree of uncertainty associated with them, and their treatment will be similar to that presented in the TSPA-VA (CRWMS M&O 1998a, Chapter 6, Section 6.5).

The mass of radionuclides in the flowing water will be determined by their form (dissolved or colloidal) and solubility limits. These properties will be treated as uncertain. They will be functions of sampled parameters as described in Sections 3.5.7 and 3.5.8. The other three quantities listed above will also be a function of uncertain variables that will be sampled in the TSPA RIP calculations. These uncertain variables and their treatment are described as follows.

The amount of water flowing through the drip shield will be a function of the amount of seepage entering the drift, the fraction of this seepage contacting the drip shield, and the breached condition of the drip shield. The amount of seepage entering the drift and the breached condition of the drip shield will be provided by the drift seepage abstraction model (Section 3.1) and the drip shield degradation abstraction model (Section 3.4), respectively. Three types of breaches on the drip shield may occur (1) crevices, (2) patches, and (3) pits. The fraction of water contacting the drip shield will be treated as an uncertain quantity and will be represented by a sampled variable. The amount of water flowing through the drip shield will be a fraction of the water contacting the drip shield. This fraction of water that flows through the drip shield will be assumed to be proportional to the fraction of the drip shield surface area that has been breached. The breached surface area of the drip shield will consist of three parts (1) the crevice area, (2) the pit area, and (3) the patch area. To account for uncertainty in the amount of water entering each part, three sampled parameters will be defined that scale the amount of water flowing through crevice, pits, and patches. The distributions representing each of these sampled variables will be defined using lab scale testing data and process model analyses.

The amount of water entering and flowing through the waste package will be treated in a manner similar to that of the drip shield. That is, sampled parameters will be defined for the fraction of water contacting the waste package (this water will be a fraction of the water entering the drip shield) and for the amounts of water entering the waste package through crevices, pits, and patches.

The amount of water flowing through the invert directly beneath the waste package will be assumed to equal the amount of water entering the drip shield plus an uncertain fraction of the difference between seepage flow into the drift and flow through the drip shield. This uncertain fraction will be represented by a sampled parameter with a defined distribution that is based on lab scale testing data and process model analyses. The liquid saturation in the invert beneath the waste package will be determined for each flow value, using a cross-sectional flow area defined by the footprint of the drip shield and the relative permeability versus liquid saturation characteristic curve for the invert medium. The calculated liquid saturation will be used to calculate an effective diffusion coefficient for diffusive radionuclide transport through the invert.

Sorption of radionuclides onto corrosion products, and possibly invert materials, may substantially retard the release of some radionuclides from the EBS. Sorption onto corrosion products will be assumed to be a linear process and represented by radionuclide specific partition coefficients (K_ds) for sorption. These K_ds will be treated as sampled parameters, with distributions that will be defined based on EQ3/6 process modeling and bounding assumptions.

3.7 SATURATED ZONE FLOW AND TRANSPORT

The SZ is the region below the water table where rock voids, pore spaces, and fractures are completely filled with groundwater. The SZ lies under the UZ, which contains the emplacement horizon selected for the potential repository. If releases from the repository occur, radionuclides in aqueous or colloidal forms could migrate through the underlying UZ, ultimately reaching the region of groundwater below the water table. Upon entering the SZ, the radionuclides are expected to be transported by the groundwater, ultimately reaching the Amargosa Valley, approximately 20 km downstream. The SZ is an important component of the natural barrier and contributes to total system performance in three fundamental ways:

- It delays the arrival of aqueous phase radionuclides at the accessible environment (increases the confinement and residence time in the geologic media) as a result of sorption and matrix diffusion.
- It provides media for filtering colloidal radionuclides through physical and chemical interactions with earth materials.
- It reduces the concentration of radionuclides as they are transported along groundwater flow paths.

The purpose of the SZ models is to provide a quantitative description of the rates and direction of groundwater flow, which in turn provides information for the estimation of radionuclide transport from the repository to the location of water used by the critical group.

For the TSPA-SR, the SZ process level models and abstractions have been developed to describe flow and transport processes controlling the fate of radionuclides that might enter the groundwater. The purpose of this section is to provide the technical basis for SZ models, including the conceptual framework and key assumptions. In addition, this section also provides a description of cases to be considered in sensitivity analyses.

3.7.1 Introduction

The SZ flow system at Yucca Mountain is in the Alkali Flat-Furnace Creek groundwater subbasin within the Death Valley groundwater flow system. The Alkali Flat-Furnace Creek groundwater subbasin 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 subbasin and along Fortymile Wash. Although there may be some limited mixing of groundwater across subbasin boundaries, hydrologic and hydrochemical data indicate that they form relatively distinct groundwater flow systems.

The SZ beneath the repository footprint includes a lower volcanic aquifer that consists of the Prow Pass, Bullfrog, and Tram formations. 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. 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. Analysis of multiwell hydraulic testing at the C-wells provides much higher estimates of hydraulic conductivity (by approximately a factor of 100) than single well tests for the same borehole intervals.

In the current conceptualization, the lateral flow of groundwater in the upper SZ beneath the repository and downgradient from the repository occurs in fractured porous volcanic rocks, transitioning to alluvium somewhere between 10 and 20 km from the repository. Interpretation of available hydraulic head measurements indicates that groundwater flow is generally to the south and east near the potential repository, transitioning to a more southerly flow farther to the south. Groundwater flow from beneath Yucca Mountain would probably be discharged to pumping wells in the Amargosa Valley, given present water use conditions in the region. Under predevelopment conditions and present climatic conditions, the ultimate discharge of groundwater from beneath Yucca Mountain probably occurs at Franklin Lake Playa and at springs in Death Valley, approximately 80 km from Yucca Mountain.

The potentiometric surface for the SZ in the immediate vicinity of Yucca Mountain indicates large variability in the magnitude of the hydraulic gradient. 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 2 km. 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. 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.

At present, there is relatively little hydrogeologic data for the alluvial portion of the flow system. However, Nye County is currently drilling and characterizing more than 20 boreholes that are expected to provide data on the alluvial aquifer. Most of these new boreholes are distributed along the 20 km boundary where the critical group is assumed to be located (see Section 3.8). Data from the new boreholes will include:

- Lithologic information
- Hydraulic heads
- Limited measurements of hydraulic conductivity
- Groundwater chemistry.

Hydrogeologic data from these new boreholes are expected to be available for use in the TSPA-SR.

Transport of radionuclides through the SZ can occur either as dissolved species or in colloidal form (most likely adsorbed to natural or wasteform colloids, or within the structure of wasteform colloids). Evidence from the C-well tests indicates that both adsorption and diffusion of radionuclides into the matrix are operable processes for solute transport. Also, the C-well tests indicated that colloidal transport can occur, although with considerable filtration or delay of a substantial portion of the colloids.

3.7.2 General Description of Process Model and Abstraction

To provide realistic flow fields representative of the unique hydrogeologic features of the Yucca Mountain site, process level models for two different spatial scales have been developed. The first flow model is a regional scale, steady state flow model (D'Agnese et al. 1997) encompassing a large portion of southern Nevada and parts of eastern California. Within this regional model is a smaller site-scale flow model encompassing the repository footprint and the flow domain that extends to the designated location of the critical group at 20 km.

The regional scale flow model considers a 275 km by 375 km region, and computes the water budget as a function of the natural system boundaries and recharge and discharge relationships. The groundwater system is conceptualized as a 3-D porous continuum composed of major, regional scale hydrogeologic units and hydrologically significant structural features. Representation of the hydrogeologic system is simplified in the regional scale groundwater flow model by combining hydrogeologic units into four major conductivity zones. Darcy fluxes and heads are the principal output of the deterministic regional-scale model, which in turn is used to set boundary conditions for the site-scale flow model.

The site-scale flow model is being developed to analyze the performance attributes of the SZ, including the flow path geometry and characteristics required for TSPA calculations. A 3-D representation of the flow system includes an area of about 30 km by 45 km. The site-scale model will be calibrated with available water level data and hydrochemical information. Deterministic site-scale flow simulations will be conducted with the FEHM computer program (Zyvoloski et al. 1996) to generate realistic flow fields by taking into account:

- Detailed 3-D geologic information

- Impact of structural control on flow (e.g., Solitario Canyon Fault, Bow Ridge Fault, Fortymile Wash, and others)

- Distributed and focused recharge

- Results from hydraulic and tracer testing within the lower volcanics aquifer.

For the purposes of modeling radionuclide transport, the groundwater system is conceptualized as a dual porosity continuum. The 3-D transport modeling will also be performed with FEHM. The FEHM streamline particle tracking algorithm will be used to simulate aqueous phase radionuclide transport processes through the SZ, including:

- Advective transport along streamlines
- Hydrodynamic dispersion
- Matrix diffusion
- Linear sorption
- Radioactive decay.

The process model for colloid facilitated radionuclide transport is presently being developed and will be simulated separately from the SZ site-scale flow and transport model. A one-dimensional transport model is being used that takes into account the above transport processes, including filtration of colloids and kinetic sorption of plutonium onto colloids, but excluding matrix diffusion. Two colloidal components are modeled (1) radiocolloids, formed by sorption of dissolved radionuclides onto natural colloids, and (2) colloidal particles produced by waste form(s).

A series of stochastic transport simulations for a unit mass flux source will be performed with the FEHM program to obtain breakthrough curves at 20 km. Transport simulations will produce a large library of unit breakthrough curves that will be used in an abstracted transport model suitable for inclusion in the computer program that will be used for the actual TSPA calculations. The convolution integral method is used to produce the model abstraction. The convolution integral method takes a radionuclide source mass from the bottom of the UZ transport model for a given timestep, and combines it with the appropriate breakthrough curve for that radionuclide, giving the masses and times that the radionuclides reach the 20-km boundary. The method is implemented for TSPA using numerical integration over the time of interest. Changes in recharge associated with climate variations will be approximated as a step from one steady-state flow condition to the next. The principal output of convolution integral method will be the mass flux (as a function of time) at the 20 km boundary for each radionuclide and for each realization.

Concentrations of radionuclides in the water supply of the critical group will be calculated in the TSPA analyses by dividing the radionuclide flux for the entire plume (reaching 20 km) by the pumping rate. This approach is consistent with the approach suggested in the proposed 10 CFR 63 (64 FR 8640). The pumping rate is expected to be typical of a farming community consisting of approximately 100 individuals; this model parameter would be treated stochastically and sampled from a specified distribution.

This method of abstraction is similar to the method used in TSPA-VA, except in 3 respects. First, the breakthrough curves for TSPA-SR will be calculated using the SZ 3-D model and will reflect the improved geology, dimensionality, and geometry that the 3-D model offers. For TSPA-VA, the breakthrough curves were calculated using six one-dimension stream tubes. Second, for TSPA-SR, dilution will be implicit in the concentration calculation where the entire mass flux is incorporated in a withdrawal volume. For TSPA-VA, a dilution factor was explicitly applied. Third, for TSPA-SR the final concentration of a radionuclide will be calculated based on the withdrawal volume. For TSPA-VA, the calculation of the final concentration involved combination of the flow tubes with a correction applied if the resulting concentration was non-physical.

3.7.3 Significant Coupling with Other Models

In making their contributions to the TSPA calculation, the SZ flow and transport models are directly linked to three other process level models. These other models include (1) the UZ flow model, which provides the recharge pattern at Yucca Mountain (see Section 3.1); (2) the UZ transport model, which provides the magnitude and distribution of radionuclide source terms (see Section 3.1); and (3) the biosphere model, which uses the SZ radionuclide concentrations to estimate the dose rate (see Section 3.8).

The SZ flow and transport models are not directly coupled to the TH model or to the disruptive scenario models. Consequently, the SZ models neglect the effects of the temperature field generated by the repository decay heat and any potential changes in the hydrostratigraphy induced by seismicity, igneous activity, and faulting. Sensitivity studies may be conducted to evaluate the effect of disruptive events on the SZ performance.

3.7.4 Major Assumptions

In developing the process level models for SZ flow and transport, the classical conservation principles of science have been used. However, a number of fundamental assumptions have been made as well. For the deterministic groundwater flow model, for instance, the following key assumptions apply:

- The flow is steady state and predominantly lateral.
- The flow system is treated as a confined aquifer.
- The hydrogeologic setting is represented by laterally discontinuous, vertically stratified, but internally homogeneous units.
- The hydraulic boundary conditions for the site-scale model are based on the regional scale-model results.
- The site-scale groundwater flow patterns are not affected by water withdrawals from a hypothetical well of the critical group.

- The changes in water table elevation and groundwater flow patterns caused by climate change (other than the change in flux) are not significant.

Similarly, for the radionuclide transport model, the following basic assumptions constrain the theoretical basis of the mathematical model:

- Hydrodynamic dispersion is a function of flow magnitude and direction
- Radionuclide sorption is reversible and described by a linear isotherm
- Mass transfer between fractures and matrix occurs as described by Fickian diffusion.

The fundamental assumptions of the convolution method, as applied in the abstraction for the TSPA calculation, are (1) steady state flow conditions exist in the SZ, and (2) transport processes are linear.

3.7.5 Implementation in Total System Performance Assessment–Site Recommendation

For the TSPA-SR, simulations of SZ flow will be performed using the 3-D SZ flow and transport model. Three flow simulations will be performed corresponding to (1) the expected groundwater flux, (2) a high groundwater flux, and (3) a low groundwater flux (see Section 3.7.6). The flow fields will be used by the transport module of the 3-D saturated zone model to generate breakthrough curves for the various radionuclides and sampled transport parameter sets. The breakthrough curves will be used by the abstraction model—the convolution integral method—in the TSPA computer program to determine radionuclide flux to the biosphere.

Climate change will be considered as part of the TSPA-SR SZ flow model. Because the analysis for the TSPA-SR will focus on a regulatory compliance period of 10,000 years, the flow and transport model will cover the sequence of future climates discussed in Section 3.1. Convolution integrals will be developed for each of these climates and for expected, high, and low groundwater fluxes. During a given realization when a climate change occurs during the simulation, the flow field is assumed to instantaneously change from one climate state to the next.

In contrast to the SZ flow model, which will produce a limited set of calculations with only the groundwater flux varied, the radionuclide transport model will be run in a stochastic mode with various transport properties treated as statistically distributed parameters. The parameters that may be statistically sampled in the 3-D calculations include permeabilities, dispersivities (longitudinal and transverse), and sorption coefficients. The location of the interface between the alluvial valley fill and the tuffs—a potentially important parameter—will be sampled from a distribution and included in the transport calculations. The base case will consider colloid facilitated transport, but only for a limited set of radionuclides that can contribute significantly to dose (e.g., isotopes of plutonium).

3.7.6 Sensitivity Cases

A series of sensitivity analyses are expected to be conducted to provide greater insights to SZ performance attributes, as well as to support the technical basis for the TSPA. A preliminary list of possible sensitivity analyses is presented below (Note that the list of sensitivity studies cannot be specified exactly until initial TSPA results can be analyzed to determine which parameters and models must be examined in greater detail):

- Determine the sensitivity of model calculations as a function of the number of source regions.
- Identify the preferential flow pathways in the SZ to determine conservative locations for specifying source regions.
- Examine alternative modeling approaches for incorporating the effects of matrix diffusion.
- Evaluate the changes in water table and groundwater flux induced by climate changes.
- Conduct geostatistical simulations to bound the dispersivities at the subgrid block scale.
- Evaluate the increase in apparent dispersion resulting from climate change.
- Examine alternative conceptual models of site-scale flow in the SZ as a function of hydraulic boundary conditions.
- Examine the impact of structural features on flow paths and groundwater velocities.
- Investigate the effects of large-scale anisotropy on regional and site-scale groundwater flow patterns.

In addition, some sensitivity analyses may be carried out to evaluate certain model assumptions and evaluate the reasonableness of selected parameters or ranges. Also, in order to show the robustness and defensibility of the TSPA, analyses could be conducted where the SZ flow and transport component in the TSPA-SR would use the 3-D SZ model, parameterized such that the behavior would maximize the dose within a 10,000-year time frame. Groundwater flux would be specified at the high end of the expected range (i.e., it will be based on the estimated upper value of the uncertainty range for the glacial transition climate). Groundwater velocity would then be calculated using a value for fracture porosity at the lower end of the range of the distribution used for the TSPA-SR. Sorption distribution coefficients for the matrix would be based on the lower ranges of the distributions used for TSPA-SR (no sorption would be assumed for the fractures). Fracture spacing for the volcanic rocks will be set to minimize matrix diffusion. The location of the volcanic/alluvium interface would be set to minimize the length of the flow path through the alluvium. Colloid facilitated transport would be modeled so that the upper bound of the fraction of irreversibly sorbed radionuclides is specified and the upper bound of the partitioning coefficient for reversibly sorbed radionuclides is used.

3.7.7 Treatment of Uncertainty

In the SZ modeling, there is uncertainty in the flow characteristics, i.e., path, velocity, exchanges between matrix and fractures, and structural control, and transport characteristics (i.e., dispersivity, sorption, matrix diffusion), and significance of colloids. There is also variability in many of these factors (e.g., the sorption affinity changes with respect to mineral changes and previous geochemical history within the SZ). For the SZ component of the TSPA-SR, uncertainty and spatial variability are treated in the same manner. Uncertain and spatially variable parameters will be specified as random quantities with associated probability distributions.

For the TSPA-SR, the basic strategy is to use the Monte Carlo method to sample from distributions, calculate realizations of possible outcomes, and combine the results into a distribution of doses. To this end, the SZ parameters will be sampled and used in the SZ model, and the model will be used to generate a series of possible flow and transport fields that can be sampled in the TSPA calculation. This method was previously used in the TSPA-VA.

To provide defensible estimates of SZ performance attributes in the TSPA, a realistic and complex conceptual model of subsurface geology has been developed by incorporating detailed (i.e., 3-D) information of the subbasin stratigraphy, a depiction of structural control on flow, and the significant recharge/discharge relationships. This realism will be preserved in the flow fields calculated for the TSPA-SR, where the only acknowledged explicit uncertainty will be the groundwater flux. Of the flow parameters that influence possible radionuclide flux to the biosphere, the groundwater flux is the most important because it directly affects the travel time and can be used as a surrogate for uncertainty in other parameters that affect the travel time (e.g., uncertainty or variability in porosity can be included in the uncertainty in flux). Also of importance from a performance perspective is the flow path, specifically how much of the flow path is in the volcanic tuffs and how much is in the alluvial valley fill. Uncertainty about the length of the flow path in the alluvium is considered in the transport modeling, discussed below. To account for uncertainty in groundwater travel time, three different groundwater fluxes will be considered high, medium, and low. Each future climate state will have three different groundwater fluxes.

For the most part, consideration of uncertainty and variability will be focused in the transport modeling. The transport parameters that are uncertain or variable, but are important to performance, will be specified by probability distributions. These distributions will then be sampled (along with the groundwater flux) to determine parameters for a 3-D flow-and-transport calculation. A flow-and-transport calculation will be performed with these sampled parameters for a unit concentration of each radionuclide to be considered in the TSPA-SR for each climate state. The parameters will then be resampled and a new set of calculations performed, until a given number of realizations are reached (e.g., 100). Each one of these calculations will produce a breakthrough curve. These breakthrough curves will form a library of possible transport futures. During the TSPA calculation, this library will be sampled to be used by the convolution integral method to calculate the radionuclide flux to the biosphere.

The transport parameters that could be specified with probability distributions include the following fracture porosities, flowing interval spacings, dispersivities, sorption coefficients, and colloid transport parameters (to be determined, but could consist of the irreversibly sorbed fraction and the colloid/solute partitioning coefficient). Work is also planned to specify the fraction of the flow path in the alluvial valley fill as a random variable, with a distribution not yet determined. During a given set of SZ calculations, the volcanics alluvium boundary location would be sampled, the material properties assigned to the 3-D model would be modified to reflect the new boundary, and the calculations would be performed. Incorporation of this boundary uncertainty will be limited to the transport calculation (any effect on flow is assumed to be negligible), but this assumption will be checked.

All the parameter values that go into each set of breakthrough curve calculations will be saved. After the TSPA calculations are completed, the SZ parameter values will then be available for use in the TSPA regression analysis.

3.8 BIOSPHERE

Radionuclides released from a repository at Yucca Mountain can only cause harm if they reach that part of the earth where living organisms reside—the biosphere. Of particular interest is the human component of the biosphere and how radionuclides might impact human inhabitants of the Yucca Mountain region. In TSPA-SR, two basic pathways that radionuclides can take to reach the biosphere will be analyzed (1) through the SZ via groundwater usage, and (2) through the air in the event of dispersal by a volcanic eruption. Within the biosphere component, there are mechanisms to both disperse and to concentrate radionuclides that the TSPA-SR biosphere modeling effort must address.

3.8.1 Introduction

The biosphere modeling for TSPA-SR will be primarily based on the model used in TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.1.1), with modifications to address comments by review groups and requirements given in proposed 10 CFR 63 (64 FR 8640). The primary measure of repository performance (as specified in proposed 10 CFR 63 (63.113 and 63.115) (64 FR 8640)) is the total effective dose equivalent (TEDE) received by a person over a 50-year period from a one year exposure to radiation. This person is an average adult member of the critical group (the hypothetical group of individuals reasonably expected to receive the greatest exposure to radioactive materials released from the repository). Further requirements from the proposed 10 CFR 63 (64 FR 8640) specify that the critical group should reside within a farming community of about 100 individuals located approximately 20 km south of the repository in the vicinity of Amargosa Valley. The behaviors and characteristics of this farming community should also be consistent with present-day conditions in the region.

From a biosphere perspective, Yucca Mountain lies in a semiarid, sparsely populated region between the Great Basin and the Mojave Desert in southern Nevada. The nearest community in the direction of flow of groundwater is Amargosa Valley, an area of approximately 1,300 km^2, defined as a tax district by the Nye County commissioners in the early 1980s. Within this district, the closest inhabitants to Yucca Mountain are approximately 20 km south at the intersection of U.S. Highway 95 and Nevada State Route 373, in the location known as Lathrop Wells. There are about eight inhabitants at this location. The closest agricultural area, and where the majority of the people live, is the Amargosa Farms area located approximately 30 km to the south of Yucca Mountain. Evaluation of water flow and wind patterns suggests that any contamination from a repository at Yucca Mountain could spread south and east into this region. The Amargosa Valley region is primarily rural in nature. Agriculture is mostly directed toward growing alfalfa; however, gardening and animal husbandry are common. Water for household uses, agriculture, horticulture, and animal husbandry is primarily acquired from local wells.

Although sparsely populated, the Amargosa Valley region does support a population of 1,270 in approximately 450 households.

3.8.2 General Description of Process Model and Abstraction

Incorporation of the biosphere component into the TSPA-SR calculations will consist of two steps. The process model step involves creating a model of the average member of the critical group (the receptor) and the biosphere pathways that might direct radionuclides to that person. The model is implemented in a qualified computer program (GENII-S) for predicting radiation dose. Model parameters will be quantified using the regional survey and data from accepted national and international sources. The model uses a unit concentration of a radionuclide in water as the input, and produces a BDCF for that radionuclide as the output. The BDCF includes the effects of various pathways through the environment (e.g., irrigation and uptake of a contaminant by vegetables, then ingestion by the receptor), as well as various pathways through the receptor (i.e., through the dose conversion factor that includes the fraction of the contaminant that is taken up by the receptor, where it is accumulated in the body, and its retention time). The BDCF is the abstraction of the biosphere process model. In the TSPA calculation, a radionuclide concentration in the groundwater (or in the case of the volcanism scenario, a concentration in the ash deposited onto the soil) is multiplied by the appropriate BDCF to determine the TEDE to the receptor. The TEDE to the receptor is then compiled as the sum of the TEDEs from all radionuclides.

3.8.2.1 Definition of the Critical Group

In order to construct a biosphere model, the receptor(s) of the contamination must be defined. Consistent with requirements from proposed 10 CFR 63 (63.115) (64 FR 8640), the TSPA-SR biosphere component will focus on the receptor being an individual living in the present-day Amargosa Valley environment. This receptor is defined as the average member of the critical group, where the critical group is composed of those individuals expected to receive the highest doses as a result of the discharges of radionuclides from a repository. The critical group is part of a hypothetical farming community of about 100 persons living 20 km from a potential repository at Yucca Mountain. The receptor is described as an adult living year-round on a farm or in a similar domicile. The person has a garden, livestock, and access to locally grown food, and consumes locally grown food in types and amounts calculated for present-day inhabitants. Also consistent with requirements from proposed 10 CFR 63 (64 FR 8640), only present-day conditions will be considered when defining the characteristics of the receptor. The community takes all water for agriculture and domestic uses from wells. Except for releases associated with volcanism (see below), contaminated well water is assumed to be the only way that radionuclides can reach the receptor.

A survey of people living in the area was completed in 1997. The survey was designed (among other reasons) to permit an accurate representation of dietary patterns and lifestyle characteristics of residents within an 80 km radiological monitoring grid surrounding Yucca Mountain. The survey was focused on the Amargosa Valley region; it also included Beatty, Indian Springs, and Pahrump. Over one thousand interviews were completed for the survey, including 43 percent of the households in the Amargosa Valley. The survey was used to define the food consumption of the receptor in TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.4.1), and will be used to define the receptor in TSPA-SR. Of special interest was the proportion of locally grown foodstuff that was consumed by local residents (i.e., irrigated with the potentially contaminated groundwater) and details of what food types were eaten on a regular basis. These frequency data were converted to estimates of annual consumption of selected foods in terms of weight. In general, a higher percentage of locally produced food is consumed by residents in the Amargosa Valley than residents in the remainder of the survey area. Thus, Amargosa Valley residents have food consumption habits that make them somewhat more susceptible to radionuclide intake through the ingestion pathway than their immediate neighbors. This supports their designation as a likely population to be included in the critical group.

For the TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.4.5.2), the average person was selected as the receptor, with habits and consumption of locally produced food taken from distributions based on all the data from the survey that came from Amargosa Valley residents. This average person consumes some locally produced food, about 1.8 L/day of tap water, and spends about 10 hours per day outdoors. Survey data for the Amargosa Valley total population resident adult was sufficient to yield statistically meaningful interpretations for parameter development. Because of its proximity to Yucca Mountain, the Amargosa Valley data subset was deemed more appropriate than the total survey area of the total population resident adult data set. Sensitivity cases for TSPA-VA also investigated arbitrarily defined receptors with the characteristics of a residence farmer and a subsistence farmer (no person interviewed in Amargosa Valley completely fit the description of a subsistence farmer). For the TSPA-SR, the intent will be to examine all the data from the survey that came from the Amargosa Valley residents to determine if there is a logical distinction that would allow a critical group to be defined within the population. If so, the receptor will be described with distributions from this subset. If not, then it must be assumed that the entire population is the critical group, and the average person will be used again in the modeling.

3.8.2.2 Process Model

The strategy used to conceptualize the Amargosa Valley environment for the TSPA-VA biosphere component (CRWMS M&O 1998a, Chapter 9), and which will also be followed for TSPA-SR, is consistent with similar activities being pursued by the international scientific community. In this regard, guidance was taken from the NRC (1995b), the Biosphere Model Validation Study II Steering Committee (BIOMOVS II 1994), and the Reference Biosphere Working Group (BIOMOVS II 1996) to develop an approach to evaluating long-term effects of radioactive waste disposal systems. For TSPA-SR, the recommended methodology for biosphere analysis developed by the international participants of the Steering Committee and the Working Group will be used.

The computer program to be used in TSPA-SR (as in TSPA-VA, CRWMS M&O 1998a, Chapter 9, Section 9.2.2.3) will be GENII-S (Leigh et al. 1993). GENII-S is a comprehensive biosphere modeling program and it includes a stochastic modeling capability. Input to GENII-S consists of parameter values that describe the receptor and the pathways through the environment to the receptor. An interaction matrix was developed to identify the features of the biosphere and the events and processes by which radionuclides move from one feature to another (CRWMS M&O 1998a, Chapter 9, Section 9.2.1, Table 9-1). Using the interaction matrix, important elements of the biosphere and the pathways among these elements have been defined. Most of the parameters used by the model define the characteristics of these elements and the pathways. Exposure pathways fall in three principal categories ingestion, inhalation, and external exposure pathways (all of which are included in the TSPA-VA biosphere model and will be included in TSPA-SR).

3.8.2.3 Abstraction

The entire biosphere can be condensed into a number that, when multiplied by the concentration of a radionuclide at the geosphere and biosphere, interface gives the all-pathway annually committed dose. This number is called a BDCF, and because it includes uncertainties in input parameters it is generated as a probability distribution. As in TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.5.4), to calculate the radiation dose incurred by the receptor in the TSPA-SR a BDCF (for a given radionuclide) is sampled from its distribution, and the sampled BDCF is multiplied by the predicted concentration of that radionuclide in well water (or, in the case of volcanism, a concentration in soil). The result is the TEDE that the receptor receives from that radionuclide at that time. The BDCFs were completely correlated in the TSPA-VA calculations (DOE 1998a, p. 3-157), and will be completely correlated in TSPA-SR (i.e., if a large BDCF is sampled for one radionuclide, then large BDCFs are sampled for all radionuclides). The sum of the annual doses for all radionuclides is the TEDE at that time. Even if this assumption of complete correlation is not correct, the expected value of the total annual dose is not affected, but the distribution of the predicted doses is artificially widened.

3.8.3 Significant Coupling with Other Models

The biosphere is the last component in the chain of TSPA components and, thus, has no output coupling. Upstream from the biosphere, there are two connections (1) for the nominal case scenario, the biosphere is coupled to the saturated zone flow and transport model; and (2) for the disruptive scenario, the biosphere is coupled to the volcanic dispersal model. As required by the proposed 10 CFR 63 (64 FR 8640), only present-day conditions are considered. Thus, the biosphere will not be directly coupled with the climate model. Climate change will be included in the dose calculations, however, through the effects of climate change on groundwater flow in the UZ and SZ.

The coupling to the SZ model is through the concentration of radionuclides in the groundwater—the water that the receptor accesses through a well. It is planned to estimate the radionuclide concentration in a manner that is consistent with proposed 10 CFR 63 (64 FR 8640). The total mass of each radionuclide to be considered in TSPA-SR will be calculated by the SZ abstracted model (Section 3.7) at a distance of 20 km from the repository for a one-year period. These masses will vary over time and they will be dependent on parameters sampled for each TSPA-SR realization. Independently, the volume of water that is used annually by a farming community of approximately 100 persons will be sampled from a predetermined distribution. The concentration will then be calculated as the mass of each radionuclide divided by the volume of water. The concentration of a given radionuclide at a given time would then be multiplied by the BDCF (the biosphere abstraction) to determine the TEDE for that radionuclide. The TEDE will include the effect of buildup of radionuclides in the soil caused by continuing irrigation (see Section 3.8.5).

How the statistical distribution of water usage volume will be defined has not yet been determined. Two possible methods are described as follows. The first method is based on the estimated present-day water usage (approximately 10^7 m^3/yr) and population (approximately 1,270) of the Amargosa Valley. A lower bound of the water usage distribution could be the set of farming families, comprising about 100 people, that use the minimum amount of water; the upper bound could be the total amount of water usage in Amargosa Valley. (Because most of the present-day water usage in Amargosa Valley is for commercial agriculture, and only a small subset of the population is engaged in this activity, it is reasonable to assume that a 100-person farming community might use virtually all of the water.) The distribution would then be uniform between these bounds. Note that the lower bound of the water usage distribution would result in the highest concentrations and the greatest TEDE.

The second method of estimating the water usage volume is based on land area. Similar to the direct water usage estimate, the area of land presently worked by farming families in the Amargosa Valley can be estimated. The lower bound might be the minimum area; the upper bound might be the average area (again, because of the inclusion of commercial concerns). These areas would be converted into water volumes using the typical volume of well water needed to farm a given area. The reason to use this method over the direct method would be that information concerning land usage might be more readily available than information concerning water usage.

The coupling to the volcanism model is through the concentration of radionuclides in the ash that is deposited on the ground. The volcanic dispersal model (Section 3.9) calculates a concentration of each radionuclide in a deposit resulting from a volcanic eruption. Following the deposition, the removal of the radionuclides by atmospheric processes will be estimated as a function of time. The concentration of a given radionuclide at a given time (i.e., deposited quantity multiplied by the removal factor and the radioactive decay fraction) would then be multiplied by the BDCF for volcanism (the biosphere abstraction) to determine the TEDE for that radionuclide at the time since deposition event. The expected dose for the volcanic scenario can then be determined by multiplying the TEDE by the event probability and integrating over time.

Combination of the TEDEs from the nominal and disruptive scenarios is discussed in Section 4.

3.8.4 Major Assumptions

The major assumptions in the biosphere component of TSPA-SR come from proposed 10 CFR 63 (63.115) (64 FR 8640) and from the generally held assumptions by the international biosphere modeling community. These major assumptions are:

- Present-day behaviors and characteristics of the critical group are representative of future behaviors and characteristics (including water usage and food consumption).

- The critical group is within a small farming community of approximately 100 persons.

- The critical group can be represented by the average adult member of the group.

- The small farming community is located 20 km south of a repository at Yucca Mountain.

- Radionuclides released from Yucca Mountain will disperse completely and uniformly in the water supply of this farming community.

- Climatic evolution can be extrapolated from the past.

- Geologic evolution can be based on what is known about natural processes.

- It is reasonable to use deterministic dose conversion factors, calculated based on the method defined by the ICRP.

- The TEDE of a radionuclide is proportional to its concentration at the interface of the geosphere and biosphere (this assumption is the basis for using a BDCF).

- A person near Yucca Mountain during a volcanic event will leave the vicinity before accruing a significant dose from the ash fall and will return upon cessation of the volcanic activity.

3.8.5 Implementation in Total System Performance Assessment–Site Recommendation

The TSPA-SR will evaluate two scenarios the nominal scenario and the disruptive scenario (volcanism). The biosphere component for the assessment of these scenarios is discussed here. The emphasis is on the differences between TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.5) and TSPA-SR.

3.8.5.1 Biosphere Model Associated with the Nominal Scenario

In addition to the guidance given in proposed 10 CFR 63 (64 FR 8640), the biosphere component would incorporate changes brought about by comments from groups that reviewed TSPA-VA. There were three general areas of the TSPA-VA biosphere component that received comments from review groups, which included the NRC, the PAPR Panel, and the DOE Management and Technical Services Contractor. These general areas are (1) pumping effects on radionuclide concentrations in groundwater; (2) effects of surface processes (e.g., erosion, chemical or biological buildup) on radionuclide concentrations in soils; and (3) the definition and location of the receptor group. In addition, the TSPA-SR will be compliant with the QA program.

Item 1: Critical Group Details–In an effort to bound the probable range of receptor lifestyles in the vicinity of Yucca Mountain, three receptors (the average Amargosa Valley resident, the residential farmer, and the subsistence farmer) were selected for the calculation of BDCFs for TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.5.2). For SR, the receptor will be the critical group that is defined in the NRC's proposed 10 CFR 63 (64 FR 8640). This group will be representative of the subset of adults who are most at risk (i.e., the critical group) while residing in a hypothetical farming community of approximately 100 residents at a specified location.

Item 2: Qualified Parameters–GENII-S requires a large number of input parameters. For TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.2.3), model parameters were not qualified due to schedule constraints; however, receptor parameters were based upon survey data while model transfer parameters came from applicable published literature. For SR, all parameters will be qualified (as per YAP-SIII.1Q, *Qualification of Unqualified Data*) or demonstrated to be accepted data in accordance with the YMP QA program.

Item 3: Parametric Values–For SR, an attempt will be made to base all parameters on data considered representative of the location of the critical group (i.e., site-specific, Amargosa Valley data will be used wherever possible). This approach was used to some degree in TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.2.3), but without Item 2 (adequate qualified parameters) this concept may not be possible for all parameters.

Item 4: Buildup of Radionuclides in Soil–For the TSPA-VA (CRWMS M&O 1998a, Chapter 9, Table 9-3), BDCFs were calculated assuming radionuclide levels in the soil arose from a single year of irrigation, in accordance with the NRC regulatory requirement for evaluating routine releases from reactors and other nuclear facilities. For SR, BDCFs will be generated and abstracted to allow the TSPA computer program to sample stochastically over both irrigation time and uncertainty bounds. Although this capability will be added, it should be noted that the radionuclides expected to contribute the most to dose during a 10,000-year regulatory period (technetium-99 and iodine-129) are not expected to have a long residence time in the soil and will not be subject to large buildup factors. The residence time of plutonium isotopes, transported via colloids, is not known.

Item 5: Radionuclide Removal from Soil–For TSPA-VA (CRWMS M&O 1998a, Chapter 9), the removal of radionuclides and soil due to erosion by wind and water was not considered, while removal due to leaching was considered. If a single year of irrigation is considered, removal by erosion is of little consequence. For the SR, the loss of radionuclides by erosion as well as leaching (taken into account in Item 4) will be considered. A model that estimates the loss of soil and associated radionuclides from soil, by erosion and leaching as a function of time, will be developed. The results of this study will be factored into the abstraction of BDCFs mentioned in Item 4.

Item 6: Radionuclide Inventory–To expedite the timely completion of Item 2 in support of the SR, the 39 radionuclides for which BDCFs were generated for TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.6.2), but not considered in the base case, will be screened to a more manageable number. This reduction should be possible as SR, in accordance with proposed 10 CFR 63 (64 FR 8640), will consider only a 10,000-year compliance period in contrast to the 1,000,000-year period considered in TSPA-VA (CRWMS M&O 1998a).

Item 7: Water Usage–As directed by the proposed 10 CFR 63 (64 FR 8640), the SR will consider a hypothetical farming community residing at or nearby Lathrop Wells (see Item 1 for the discussion of the proposed receptor). Radionuclide concentrations will be generated in the TSPA computer program by diluting the total annual mass flow of radionuclides across the 20 km boundary (calculated by the SZ model) and dividing this mass equally by the anticipated annual volumetric groundwater usage by the farming community. The TSPA-VA calculations

(CRWMS M&O 1998a, Chapter 9, Section 9.3.3.3) had all groundwater being drawn from the midpoint of the plume (i.e., the point of maximum concentration).

3.8.5.2 Biosphere Model Associated with Volcanic Activity

The biosphere model for volcanism consists of the receptor returning to the region soon after the eruption, and to live on and farm the contaminated volcanic soil. This scenario is virtually the same as the volcanism scenario evaluated for TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.5.5). The biosphere model used to evaluate the volcanic scenarios involves the same biosphere pathways model and receptor parameters as being developed for the nominal scenario.

In the volcanism scenario, it is assumed that the ash from the eruption affects the upper 15 cm of the ground surface, because this depth is representative of a plow depth and encompasses the root zone of most agricultural plants. For these calculations, the groundwater is not considered to be contaminated because this factor has already been taken into account in the nominal scenario BDCFs calculations. As with the nominal scenario, the BDCFs include the ingestion, inhalation, and external exposure pathways. As with the nominal scenario, the dominant pathway is the ingestion of contaminated foods. To determine the dose rate in a TSPA calculation, it is necessary to determine the amount of radionuclides expelled by a volcanic event and the area over which the radionuclides are dispersed. These two parameters allow the concentration of radionuclide in the soil to be calculated. The concentration of radionuclides in the soil is then multiplied by the volcanic BDCFs to give the TEDE.

Note that the volcanism scenario involving a receptor in the vicinity during a volcanic eruption will not be considered for TSPA-SR, because it is assumed that the local inhabitants will leave the area before accruing a significant dose. The dose rate associated with inhalation and external exposure during the volcanic event itself will be addressed in additional studies if it is deemed that volcanic activity requires further consideration.

3.8.6 Sensitivity Cases

For TSPA-SR, as in TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.7), a number of separate analyses will be performed to investigate the effect of the more extreme parameter values on the TSPA results. For the biosphere, the 5th and 95th percentiles of the BDCFs will be used in these sensitivity calculations. In addition, there are several other comparative analyses that might be performed to examine the impact of assumptions. The following list is presented to indicate sensitivity studies that are being considered; it is possible none of these sensitivity cases will be analyzed.

- The effect of changing the receptor to fit the definition of a reasonably maximally exposed individual could be analyzed. The reasonably maximally exposed individual concept is familiar to the international community and other government regulatory agencies. In TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.7.3), it was found that a subsistence farmer could receive a radiation dose from neptunium-237 approximately five times greater than that received by an average inhabitant of the region; however, the dose is radionuclide dependent, and some radionuclides resulted in a greater range in doses.

- It is possible that the critical group, as well as the average adult member of the group, could be defined in more than one-way. If so, analyses could be conducted to examine the impact of these differences on the final TSPA results.

- Changes in the behavior and characteristics of the critical group caused by climate change could be evaluated. A survey of the inhabitants of a cooler and wetter locale, Lincoln County, Nevada, has been completed, and if necessary, results of this survey could be used to define the habits of a critical group for a future climate.

- Rather than dissolve radionuclides completely in the water supply of a farming community in order to calculate dilution, it is possible to directly calculate the radionuclide concentration in the contaminant plume, and it could be of interest to examine what difference this method makes in the final TSPA results.

- To determine the full extent of the possible range of the BDCF parameters, calculations can be performed with the 5th percentile values of all the parameters and the 95th percentile values of all the parameters.

- The TEDE received by a person staying near Yucca Mountain during a volcanic event could be calculated.

3.8.7 Treatment of Uncertainty

Much of the biosphere component is prescribed (e.g., the location and the size of the farming community that uses potentially contaminated water, who in the critical group should be modeled, how to surmise the habits and behaviors of this person), but there are still uncertainties associated with calculating a radiation dose for TSPA-SR. These uncertainties are primarily within the process model parameters (and carried through the abstraction).

3.8.7.1 Uncertainty in GENII-S

The GENII-S model uses a Monte Carlo method to incorporate uncertainties in input parameters. The parameters can be defined by probability distributions, from which discrete values are sampled for each calculated realization. In TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.6.2), 130 GENII-S realizations were performed to define each BDCF for each radionuclide. The output doses from a GENII-S calculation (the BDCFs) were in the form of probability distributions. The distributions that these output data formed were shown to be approximated, in a statistically meaningful sense, by a lognormal distribution for input into the TSPA calculation. During the TSPA-VA calculations (CRWMS M&O 1998a, Chapter 9, Section 9.1.1), the actual BDCFs used to change radionuclide concentrations into TEDEs were sampled from the appropriate lognormal probability distributions. In this manner, the uncertainty in the biosphere component was incorporated in the TSPA-VA results. Although some of the details might change (e.g., the number of GENII-S realizations), it is planned that the TSPA-SR will incorporate biosphere uncertainties in the same way.

3.8.7.2 Parameter Uncertainty

The GENII-S computer program allows input of probability distributions to describe many important parameters. It is expected that the same parameters used in TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.2.3) will be defined probabilistically for TSPA-SR (plus water usage, discussed above) and used directly in the TSPA calculation.

The consumption rates for drinking water, vegetables, fruit, grain, beef, poultry, milk, and eggs were estimated from the results of the survey. Data on the transfer factors for local food types are limited; therefore, generic food transfer factors were taken from literature sources. Inhalation exposure, as well as direct external exposure, is dependent on the amount of time the receptor spends outdoors. The external and inhalation exposure mass load is the amount of material (e.g., dust) in a given volume of outside air. The home irrigation rate is the water application rate to lawns. The soil-to-plant uptake parameter does not reflect the soil properties of the area surrounding Yucca Mountain, but, rather, a more generalized temperate soil. An effort is being made for TSPA-SR to determine values more representative of the Yucca Mountain region.

As is the usual practice for radiological compliance evaluations, dose conversion factors (not to be confused with the BDCF) used in the biosphere model were assigned constant values. A dose conversion factor converts an amount of a radionuclide into a radiation dose, taking into account such effects as the uptake of a radionuclide by the body, the residence time for a radionuclide in the body, and where a radionuclide is concentrated in the body. It is not planned to examine the effects of using different dose conversion factors in TSPA-SR. Although different agencies and different international organizations support different values for dose conversion factors, and although it is generally acknowledged that there is uncertainty in dose conversion factor values that are not captured by a single value, it is beyond the scope of TSPA-SR to add any information to this area. The values used in the biosphere modeling will be derived using an accepted international methodology.

Analysis of the results of TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.7.3.2) for the biosphere modeling shows that the most important pathway in the calculation of the BDCFs is typically the drinking-water-ingestion pathway. The next most important pathway is the leafy-vegetable-ingestion pathway. The meat-ingestion pathway is important for iodine-129. This prioritization resulted from a deterministic calculation that used the expected values of all parameters (CRWMS M&O 1998a, Chapter 9, Section 9.7.3.2). A similar analysis will be performed for TSPA-SR. The analysis might be expanded to examine pathways important to more extreme values of important parameters.

3.8.7.3 Uncertainty Analyses

For the TSPA-VA (CRWMS M&O 1998a, Chapter 9, Section 9.7.3.2), the rank regression technique was employed to understand which input parameters were most responsible for the variance in the BDCF distributions. Of the uncertain or variable parameters that most affect the BDCFs, the leafy-vegetable and drinking water consumption rates were found to be the most important. For iodine-129, the beef consumption rate, and, to a certain extent, the milk consumption rate, were also found to be important. Parameters that are identified as the next in importance are the crop interception fraction and the crop resuspension factor. For TSPA-SR, the same technique will be used. The results of this type of analysis can be used to identify the factors driving uncertainty of the model output and determine where attention should be focused in the future.

3.9 DISRUPTIVE EVENTS

3.9.1 Introduction

As discussed in Section 2.2, disruptive events include those events and processes over the life of the repository that may cause an off-normal response by the repository systems. These systems include both the engineered components and the natural barriers. Disruptive events have a probability of occurrence over the repository performance life of less than 1.0. Those events or processes that are sure to occur are expected (i.e., have a probability of 1.0) and, therefore, are included in the nominal scenario analyses.

In the TSPA-VA (CRWMS M&O 1998a, Chapter 10, Sections 10.4, 10.5 and 10.6), four potentially disruptive events were considered igneous activity, seismic activity, nuclear criticality, and human intrusion. For the TSPA-SR, these events are being reexamined. Their status is as follows:

- An evaluation of igneous activity probabilities has been done in the *Probabilistic Volcanic Hazard Analysis for Yucca Mountain, Nevada* (CRWMS M&O 1996a, Section 4.0). The findings reported in probabilistic volcanic hazard analysis give a range for probabilities of a dike intersecting the repository from approximately 10^{-6} to 10^{-3} over 10,000 years (CRWMS M&O 1996a, Figure 4.1a). (The mean probability over 10,000 years is 1.5×10^{-4}.) Thus, the probability of igneous activity is above the level of regulatory concern, and it remains a disruptive event in TSPA-SR. Some aspects of the consequence analyses are being redone for TSPA-SR.

- The probabilities of seismic effects (ground motion and fault displacement) have been evaluated in the *Probabilistic Seismic Hazard Analyses for Fault Displacement and Vibratory Ground Motion at Yucca Mountain, Nevada* (CRWMS M&O 1998c, Sections 7.0 and 8.0). Hazard curves relating the magnitude of earthquakes to their annual frequency of occurrence have been developed in this work. There is a relatively high annual frequency of occurrence for small earthquakes and a much lower frequency for large ones. Some work is needed to develop parameters for the geologic consequences of seismicity and structural deformation that will be used for TSPA-SR.

- The probability of nuclear criticality has not been quantified to the same extent as igneous or seismic FEPs. Scoping and bounding estimates of both the probability and consequence for several criticality scenarios indicate that both are quite small (DOE 1998a, Volume 3, Section 4.4.4.3). It is expected that a more comprehensive FEP screening analysis will show that criticality can be excluded from TSPA-SR.

- Human intrusion is a disruptive event for which the NRC requires analysis in a manner that differs from all other FEP analyses. Because of the difficulty of forecasting future human technology, social and economic conditions, or institutions, a probability for the occurrence of human intrusion cannot be estimated. The NRC has, therefore, required that a stylized human intrusion scenario supplement the TSPA analyses to measure the relative robustness of the repository system to such a disruption.

- Water table rises due to various causes have been proposed in the past as potentially disruptive events for the Yucca Mountain repository, although they were not explicitly treated as such in the TSPA-VA (CRWMS M&O 1998a, Chapter 10). Water table rises due to climate change will be included in the TSPA (see Section 3.7.6). Water table rises from other causes (e.g., seismic activity) have been shown to be inconsequential with respect to overall system performance. These determinations will be documented through the FEP described in Section 2.2.

As a result of preliminary FEP screening and the TSPA-VA (CRWMS M&O 1998a, Chapter 10, Section 10.4-6) analyses, only one type of event (igneous activity) will be considered disruptive in TSPA-SR analyses. Seismic activity will be incorporated into the nominal scenario. Detailed discussion of the FEPs for nuclear criticality will be covered in an update of the *Disposal Criticality Analysis Methodology Topical Report* (CRWMS M&O 1998e, Chapter 5). It is expected that criticality will be screened out of TSPA-SR analyses based on low probability or low consequence. Human intrusion will be analyzed as a stylized scenario, as discussed in Section 4.7. A discussion of FEP screening is given in Section 2.2.

The NRC has developed a series of IRSRs that identify Key Technical Issues with regard to evaluating the suitability of a geologic repository. Those technical issues most relevant to disruptive events are listed in Table 3.9-1. Not all of these Key Technical Issues are addressed by the disruptive events analyses. Some Key Technical Issues are addressed as part of the PMRs, and others are addressed in the TSPA analyses.

Table 3.9-1. List of NRC Key Technical Issues and Subissues Relevant to Disruptive Events

	Container Life and Source Term (NRC 1998b)
CLST1	Effects of Corrosion on the Lifetime of the Containers and the Release of Radionuclides to the Near-Field Environment
CLST2	Effects of Materials Stability and Mechanical Failure on the Lifetime of the Containers and the Release of Radionuclides to the Near-Field Environment
CLST3	Rate of Degradation of SNF and the Rate at Which Radionuclides in SNF are Released to the Near-Field Environment
CLST4	Rate of Degradation of High-Level Waste Glass and the Rate at Which Radionuclides in High-Level Waste Glass are Released to the Near-Field Environment
CLST5	Design of Waste Package and Other Components of the Engineered-Barrier System for Prevention of Nuclear Criticality
CLST6	Effects of Alternate Engineered-Barrier System Design Features on Container Life and Radioactive Release from the Engineered-Barrier System
	Evolution of the Near-Field Environment (NRC 1997b)
ENFE1	Effects of Coupled THC Processes on Seepage and Flow
ENFE2	Effects of Coupled THC Processes on Waste-Package Chemical Environment
ENFE3	Effects of Coupled THC Processes on Chemical Environment for Radionuclide Release

Table 3.9-1. List of NRC Key Technical Issues and Subissues Relative to Disruptive Events (Continued)

Container Life and Source Term (NRC 1998b)	
ENFE4	Effects of THC Processes on Radionuclide Transport Through Engineered and Natural Barriers
ENFE5	Coupled THC Processes Affecting Potential Nuclear Criticality in the Near-Field
Igneous Activity (NRC 1998c)	
IA1	Probability of Future Igneous Activity
IA2	Consequences of Igneous Activity Within the Repository Setting
Radionuclide Transport (NRC 1999)	
RT1	Radionuclide Transport Through Porous Rock
RT2	Radionuclide Transport Through Alluvium
RT3	Radionuclide Transport Through Fractured Rock
RT4	Nuclear Criticality in The Far-Field
Repository Design and TM Effects (NRC 1998d)	
RDTME1	Implementation of an Effective Design Control Process Within the Overall QA Program
RDTME2	Design of the Geologic Repository Operations Area for the Effects of Seismic Events and Direct Fault Disruption
RDTME3	TM Effects on Underground Facility Design and Performance
RDTME4	Design and Long-Term Contribution of Repository Seals in Meeting Postclosure Performance Objectives
Structural Deformation and Seismicity (NRC 1998e)	
SDS1	Faulting
SDS2	Seismicity
Structural Deformation and Seismicity (NRC 1998e) (continued)	
SDS3	Fracturing and Structural Framework of the Geologic Setting
SDS4	Tectonics and Conditions
Thermal Effects on Flow (NRC 1997a)	
TEF1	Sufficiency of TH Testing Program to Assess Thermal Reflux in the Near-Field
TEF2	Sufficiency of TH Modeling to Predict the Nature of Thermal Effects on Flow in the Near-Field
TEF3	Adequacy of TSPA With Respect to Thermal Effects on Flow
Total System Performance Assessment and Integration (NRC 1998a)	
TSPAI1	Demonstration of the Overall Performance Objective
TSPAI2	Demonstration of Multiple Barriers
TSPAI3	Model Abstraction
TSPAI4	Scenario Analysis
TSPAI5	Transparency and Traceability of the Analysis

3.9.2 Igneous Activity

Important Issues–The NRC has identified several Key Technical Issues in the igneous activity IRSR (NRC 1998c, Sections 4.1 and 4.2) related to both the probability of igneous activity and its consequences to a geologic repository. The thrust of the NRC concern for igneous activity is to ensure that the risk of igneous activity is not underestimated in TSPA analyses. The PAPR, in contrast, considers igneous activity to make only a minor contribution to repository risk and believes only minimal additional effort should be devoted to analyses (Whipple et al 1999, pp. 111 through 112). An understanding of the geologic model for igneous activity is necessary to appreciate the issues of concern to the NRC and the PAPR. These assumptions are summarized here. The important issues will be detailed in the tectonic hazard PMR.

Igneous activity is a process relevant to repository performance because of the geologic setting. Basaltic igneous activity in the area followed the cessation of major silicic caldera formation and has occurred within the last million years, to the west of the repository at Crater Flat. Based on geologic evidence, if there is a recurrence of volcanic activity, basaltic magma is considered most likely to rise as small dikes in the Crater Flat area east of Bare Mountain and west of Yucca Mountain. Assumptions regarding magma generation mechanisms and structure in the deep crust do not impact performance calculations, though they are discussed in the *Probabilistic Volcanic Hazard Analysis for Yucca Mountain, Nevada* (CRWMS M&O 1996a).

Because of dike propagation pressure, it is assumed that a dike reaching a depth of 300 m below ground level will continue rising to the surface, producing an eruptive feature. When dikes reach shallow depths, magma flow often becomes concentrated in a small number of conduits representing a path of least resistance to the surface. Conduit formation may occur at any point along a dike and, thus, may (or may not) intersect the repository. Magma is expected to begin fragmentation into ash particles as it degasses upon eruption into the drifts. Interactions of magma with waste packages and their contents are considered in the waste entrainment model for the erupting volcanic plume.

The general type of future volcanic eruption in the Yucca Mountain region is assumed to be strombolian, a type of volcanic eruption that has a range of violence and dispersivity characteristics but is typically moderate. Eruptive plume characteristics, combined with wind patterns, will cause a dispersal pattern that can result in radionuclide exposure to a critical group. The critical group will have the same location as that for the groundwater pathway, 20 km to the south.

3.9.2.1 Igneous Activity Processes

Prior work has identified potential igneous activity release mechanisms relevant to the Yucca Mountain region. In the TSPA-VA (CRWMS M&O 1998a, Chapter 10) and other prior TSPAs, some mechanisms have been investigated. Scenario development work using the approach described in Section 2.2 has shown that the range of igneous activity can be captured by modeling three general types of volcanic disruptions direct release, enhanced source term, and indirect effects.

The geologic consequences of igneous activity will be analyzed in two broad areas (1) intrusive and (2) extrusive. The case receiving the most detailed effort will be an extrusive event, wherein a vent erupts through the repository, dispersing waste in the eruption. Examples of intrusive effects include interactions between magma and waste packages and waste forms that could result in increased mobilization and transport of radionuclides by groundwater. In the TSPA-VA (CRWMS M&O 1998a, Chapter 10), this analysis was called the enhanced source term. Other intrusive events are indirect effects of igneous activity on a repository. These include the formation of a dike or sill in the groundwater flow field that could alter the transport of radionuclides to the critical group.

Direct Release–This case considers the direct transport of waste to the ground surface from the repository in a volcanic eruption. Waste reaches the surface as contaminants in erupted materials. Both liquid magma (lava) and ash are possible from eruptions at Yucca Mountain. Whereas a lava flow would be expected to be confined to the vicinity of the volcano, an ash plume can be dispersed by winds over much greater distances. Thus, an ash plume has a greater chance to directly affect a large number of people, so this scenario is being analyzed. Furthermore, the critical group for dose effects is specified to be located 20 km south of the eruption, outside the region that is expected to be affected by a lava flow. Other direct release cases are retained in the FEPs list until they can be analyzed or screened out.

The analysis for the TSPA-SR postulates that igneous activity in the Yucca Mountain region results in magma intersecting the repository and an eruption occurs through the repository. It is assumed that the magma can destroy most of the waste packages that it contacts, and the waste is entrained to the surface. The eruption creates an ash cloud that is contaminated by the waste. The contaminated ash is deposited where a critical population can be exposed to the radiation. Each of these processes is represented by a range of parameter values expressed as probability distribution functions. Figures 3.9-1a and 3.9-1b illustrate the conceptual model sequence of events.

Enhanced Source Term–An igneous intrusion that reaches the repository can erupt, but it can also travel down the drifts and remain underground. In the latter case, in addition to those waste packages in the eruptive conduit, other packages can be damaged. Waste packages that are breached by the igneous intrusion, but are not within the conduit, expose waste that remains underground. Groundwater can mobilize the waste (which may be more exposed or altered in comparison with nominal conditions). The radionuclides are transported by groundwater flow through the UZ and the SZ to the critical group. For the TSPA-SR, this analysis will be similar to that done for the TSPA-VA (CRWMS M&O 1998a, Chapter 10).

Indirect Effects–Igneous activity in the area surrounding the repository can produce intrusive features or structures that can affect the repository. A dike or sill that forms in the SZ, either upgradient or downgradient from the repository, could alter the flow of groundwater. Flow alterations that occur downgradient from the repository can divert groundwater that may contain waste from the repository. Such diversion could increase the concentration of contaminants received by a critical group. The TSPA-VA (CRWMS M&O 1998a, Chapter 10) showed insignificant consequences from this case. The FEP screening activity will develop the justification for not including indirect effects of igneous activity in the TSPA-SR.

3.9.2.2 General Description of Process Models and Abstractions

Igneous Activity Processes–The geologic model forming the basis for assumptions relevant to igneous activity is the same for SR as it was for the TSPA-VA (CRWMS M&O 1998a, Chapter 10). For SR, both the probability and consequence models will be reviewed to provide better documentation and justification for the parameters used.

Probability of Occurrence–Because of the proximity of the Quaternary Crater Flat cinder cones to the YMP, the frequency of volcanism at the repository is thought to be greater than the background frequency characteristic of the Basin and Range province. Annual frequencies of occurrence of a dike intersecting the repository have been evaluated in the *Probabilistic Volcanic Hazard Analysis for Yucca Mountain, Nevada* (CRWMS M&O 1996a). To apply the probability distribution from probabilistic volcanic hazard analysis to the direct release analysis, the probability of an eruption through the repository, given a dike intersection, must be computed. This work will be done in the tectonic hazards PMR by using the *Probabilistic Volcanic Hazard Analysis for Yucca Mountain, Nevada* (CRWMS M&O 1996a) frequency distribution and by interpreting the various models for volcanism put forth by the experts.

Number of Waste Packages Hit by an Eruption–The distribution of locations of dikes in the vicinity of the Yucca Mountain repository is based on work done in the *Probabilistic Volcanic Hazard Analysis for Yucca Mountain, Nevada* (CRWMS M&O 1996a). Given that a dike intersects the repository footprint, the location of a vent on that dike relative to the repository location is also determined from probabilistic volcanic hazard analysis. For eruptions that occur inside the repository, the number of waste packages contacted by the ascending magma is a function of the conduit size, the dike orientation, and the layout of waste packages in the repository.

Magma Interactions with the Repository–Strombolian eruptions typical of those that could occur in the Yucca Mountain region range from fairly docile to violent. It is the latter type, called violent strombolian, that could disperse repository waste in an eruptive ash cloud a significant distance. The fraction of time that eruptions would be in a violent phase is not known for future igneous activity at the Yucca Mountain region. This parameter of the volcanic model will be developed as part of the tectonic hazards PMR.

The presence of repository drifts can potentially alter the propagation of a dike. The dike moves through rock because the pressure in the liquid magma exceeds the fracture strength of the rock. When the dike reaches the stress-altered rock surrounding the drifts, the mode of propagation could change, redirecting the propagation either away from the drifts or toward them. If a dike does reach a drift, whether open or backfilled, the driving pressure can be relieved. This potentially explosive decompression of the magma can fill portions of the drift with magma or ash. Further upward propagation of the dike will depend on the reestablishment of an ascent path. The location of the continuation of the dike may be removed from the point of entry of the dike into the drift. Such an offset can potentially expose more waste packages to magma than would occur if the dike propagated straight through the drifts. Comparing the geometry of a dike intersecting the repository with the repository layout that will provide information on the number of waste packages that might be contacted by magma.

Waste Package and Waste Form Degradation–The behavior of waste packages in repository drifts exposed to magma is unknown. It is expected that waste packages exposed to magma will eventually be destroyed. The strength of waste packages in a magmatic environment will be discussed in the tectonic hazards PMR. If the period of violent eruption is sufficiently long to allow the waste package degradation processes to occur, then waste packages directly contacted by ascending magma or pyroclasts would be completely destroyed and their contents entrained.

Mechanisms for waste package destruction arise from magmatic heat, chemistry, and pyroclast formation and include internal pressurization, plastic deformation of the waste package walls, corrosion, and erosion or ablation of the waste package walls. At magmatic temperatures, the pressure of the gas contained in the waste package increases, with a major contribution made by the venting of gas contained in the reactor fuel pins. This occurs because the fuel pin cladding fails at sufficiently high temperatures. The increased internal pressure may be sufficient to exceed the tensile strength of the metal end plates of the waste package.

The temperature of the basaltic magma is probably not high enough to melt the waste package walls, but it could significantly reduce their structural integrity. Once the internal pressure has been relieved, the waste package walls may collapse from the static and dynamic loads produced by the magma and from the weight of the metal waste package walls.

To model waste package failure in a magmatic environment, the time histories of the various degradation processes will be investigated. These histories will depend on waste package materials properties, magmatic environment—both intrusive and eruptive (e.g., temperature, physical form, chemistry)—and waste package prior degradation. The failure time histories can be presented as probability distribution functions for use in abstracted analyses by relating the times for degradation to the duration of violent magmatic activity. The analyses will be developed for the tectonic hazards PMR; probability distribution functions will be developed as part of the abstraction done for TSPA-SR analyses.

The magmatic environment can be very corrosive, because magma can contain reactive gases, including water, CO_2, SO_x, and H_2S. The ascending magma or pyroclasts that hit the waste package can erode the surface. The combination of plastic deformation, corrosion, and erosion is expected to eventually cause the waste package material to be removed. The waste will then be exposed to the pressure and abrasion of high-velocity magmatic gases, liquids, and particles in the ascending conduit flow. These processes will be analyzed in the tectonic hazards PMR supplemented by conservative assumptions regarding waste form behavior in the magmatic environment.

The waste form would be exposed to thermal and mechanical shocks and a corrosive chemical environment during magmatic activity, making it likely that the waste would be pulverized. Waste form particle size and size distribution following magmatic degradation are important factors in determining the extent of entrainment and subsequent dispersal of waste in the eruption. As stated above, conservative assumptions describing waste form behavior will be made in lieu of a full-scale analysis.

Waste that is contacted by magma can be considerably altered by the thermal, chemical, and mechanical environment. Changes include dissolution of UO_2 (and the associated impurities) in basaltic magma, formation of secondary phases, and vaporization of those species with low boiling points. During cooling, thermal and mechanical stresses can crack the contaminated basalt to increase contact with water. All of these processes can contribute to increased mobilization of the radionuclides that are transported by groundwater. (The analyses developed for the TSPA-VA (CRWMS M&O 1998a) on this topic will be used for the TSPA-SR.)

Entrainment of Waste–Waste can be carried to the surface in an ascending magma or pyroclast conduit if the ascent velocity is greater than the settling velocity of the waste. The latter depends on the relative densities of the waste and magma, the sizes of the waste and pyroclast particles, and the gas pressure in the conduit. The likely maximum dimension of spent fuel particles is about 1 cm, with a lower bound for particle size near 10 μm. The smaller sizes result from greater burnup in the reactor or from large mechanical or thermal stresses. Pyroclast sizes used in the TSPA analyses will be based on the judgment of volcanologists. These processes will be analyzed in the tectonic hazards PMR.

Dispersal of Waste–Dispersal of waste can occur by the air pathway or the groundwater pathway. Waste that is incorporated in the eruption will be dispersed. If the erupted waste material is in the form of ash particles (likely during any violent eruptive phase), the waste can be carried great distances from the site of the eruption. Dispersal by volcanic eruption depends on the characteristics of the volcano—the volume of ash erupted, the duration of the eruption, and the energy of the eruption—and on the physical properties of the erupted material. The wind direction and velocity are also factors. Deposition thickness of contaminated ash at any point in the vicinity of the volcano can be modeled. Transport of radionuclides from the enhanced source term uses the same modeling as that for the TSPA-SR nominal case and will not be discussed further here.

Dose Impacts–Contaminated volcanic ash deposited in ashfall from a volcanic eruption can produce doses to the critical group in several ways. The situation considered for the TSPA-VA (CRWMS M&O 1998a, Chapter 10) and TSPA-SR analyses considers a population that returns after the end of the eruption to an area where the soil is covered with volcanic ash and radioactive waste particles, and the population uses this land for agricultural and other purposes. Another scenario—where people remain at the site in the path of the eruption—is possible, but as discussed in Section 3.8, will not be considered for the TSPA-SR. The eventual removal of contaminated ash by wind and water after its deposition will be included in the tectonic hazards PMR.

3.9.3 Seismic Activity

The TSPA-VA (DOE 1998a, Section 4.4.3) analyses investigated the consequences of seismically induced rockfall on waste packages. The *Probabilistic Seismic Hazard Analyses for Fault Displacement and Vibratory Ground Motion at Yucca Mountain, Nevada* (CRWMS M&O 1998c, Sections 7.0 and 8.0) provided information for the ground motion model used in the analyses. The TSPA-SR will use hazard curves and geologic data (e.g., fault descriptions) from the probabilistic seismic hazard analyses to develop measures for several seismic effects, including ground motion damage and fault-displacement damage.

Important Issues–Seismicity and structural deformation are listed as NRC Key Technical Issues. The TSPA-SR will address these issues, as well as others that are related to them, in response to comments from technical reviews of past TSPA analyses by the NRC and PAPR Panel. The NRC has issued several IRSRs that apply to seismicity and structural deformation issues. Table 3.9-1 lists them for both seismic and igneous activity. The geologic conceptual model and resulting geologic hazards that can have repository performance consequences are the underlying reasons for study of the Key Technical Issues of concern to the NRC and others, and are described in the next section.

The PAPR comments on the TSPA-VA (CRWMS M&O 1998a, Chapter 10) noted that the analyses postulated reasonable arguments for minor impacts from seismicity that would lead to groundwater level rise, flow field disruption, and effects of fault displacement. The PAPR stated that the supporting analyses were only scoping or screening in nature and, will require a documented, convincing rationale (Whipple et al. 1999, p. 108). The PAPR's comments regarding rockfall analysis cited the same need for stronger technical support, stating that the analysis was well planned and structured appropriately, but that the analysis of the first 10,000-year period had not been done adequately (Whipple et al. 1999, p. 108). The PAPR stated that a more carefully explored analysis of this time period was needed to support the conclusion that the effect on offsite doses is minor.

General Description of Process Models–The geologic conceptual model and resulting geologic hazards relevant to seismicity and structural deformation are described in detail in the *Probabilistic Seismic Hazard Analyses for Fault Displacement and Vibratory Ground Motion at Yucca Mountain, Nevada* (CRWMS M&O 1998c, Volume 2, Appendix E). Ground motion as a consequence of seismicity is the primary process to be analyzed. Structural deformation includes the geologic consequences of movements on faults that either intersect the repository or are very close to it.

The assumptions for the seismicity and rockfall model are as follows. Backfill initially covers the waste package and drip shield with a thin layer of crushed rock. Subsequent thermal and mechanical stresses (settling or ground heave) can result in exposure of the drip shield. Ground shaking can cause rockfall in drifts. The extent and severity of the rockfall depends on the earthquake magnitude and the strength of the rock above the waste packages. In addition to direct damage to drip shields or waste packages, drift infilling from rockfall could lead to increased thermal insulation and modified water pathways, all of which could lead to increased corrosion rates for drip shields or waste packages. Another potential effect is the separation of the drip shields due to groundmotion.

Drift Collapse Model–Both thermal and seismic effects are considered drivers for rockfall. A static probabilistic keyblock analysis will provide the probability of rockfall and rock size distribution as a function of time. The analysis can also provide the probabilities of multiple rockfalls on a single waste package that could lead to additional damage. Inputs to this model include the frictional (friction angle and cohesion) and statistical characteristics (e.g., distribution of joint orientations, spacings, etc.) of each joint set. The keyblock analysis can predict unstable blocks in the roof of the drifts and, from this analysis, the probability that a block of a given mass will fall can be calculated. The keyblock analysis is static, however, and cannot take into account the shaking due to an earthquake. The static analyses will be supplemented by conducting a set of dynamic analyses of the underground drifts.

Waste Package Damage Model–The drift collapse model provides inputs to the waste package model that will combine the rock size information with waste package wall thinning to determine the extent of damage. The waste package model will calculate waste package thickness as a function of time. Waste package stresses resulting from rockfall sizes will be compared against the stresses that can cause waste package failure, no failure, or something in between. Failure can be either through a crack in the waste package or at a site for accelerated localized corrosion. Rockfall and corrosion damage are both expected to be included in the waste package degradation model for the TSPA-SR, at least in sensitivity study, as discussed in Section 3.4. The most extreme instances of rockfall (e.g., those that could occur from large magnitude earthquakes) will be investigated as potentially disruptive events.

Fault Displacement Damage Model–Fault displacement can put stresses on the waste package and drip shield that can accelerate failure. Proximity of the waste packages to the fault displacement affects the extent of damage. The repository design incorporates adequate setback of canisters from known faults so that there is reasonable assurance that direct damage by fault displacement will be negligible (YMP 1997, Section 4.2.1). New or undetected faults could occur where waste packages are located. The offset between the rock walls bounding a fault is expected to be small as a result of a fault displacement event (CRWMS M&O 1998c, Volume 2, Appendix E), but the shear stress transferred directly to a waste package or drip shield in a backfilled drift could be sufficient to cause damage. Additionally, fault displacement could produce the following hydrologic effects alteration of groundwater flow in fractures in the UZ (which could affect seepage), alteration of groundwater flow in the SZ, localized changes in rock permeability due to strain, and change in water table elevation.

3.10 TOTAL SYSTEMS PERFORMANCE ANALYSIS MODEL ARCHITECTURE

This section describes the model architecture of the total system (or TSPA) model, which combines all the different component models described in Sections 3.1 through 3.9. For the TSPA-SR, a probabilistic simulator like RIP (Golder Associates Inc. 1998) will be used as the integrating shell for linking various component codes and models together for conducting TSPA calculations. RIP uses Monte Carlo sampling of the various uncertain parameters and alternative models to derive the range of probable repository behavior through time, based on the output of the various component models through time. The different ways in which RIP represents a component model are:

- Response surfaces in the form of multidimensional tables representing the results of modeling with detailed process models.

- Functional or stochastic representations of a component model embedded directly into RIP.

- Mixing cells, which are equivalent to equilibrium batch reactors (coupled by advective and diffusive connections) that facilitate representing certain THC processes in the EBS.

- Direct coupling of process codes to RIP as external callable routines.

In the first coupling method—response surfaces—most of the computational work for the individual components of the system is done outside RIP prior to running the actual total system computations. The results from the modeling of these individual components are abstracted as multidimensional tables into RIP. An example of this method would be the abstraction of the near-field thermodynamic environment, modeled using the computer code NUFT, into RIP in the form of temperature and relative humidity time histories as a function of climate, location in the repository, waste type, and time. An example of the second method is the representation of radionuclide solubilities or concentration limits directly in RIP. The transport of radionuclides in the EBS is an example of the RIP mixing cell algorithm, and is modeled by linking a series of mixing cells together, which is mathematically equivalent to a network of finite difference nodes. The last method—coupling external functions to RIP—enables information transfer in real time at every time step. An example of this would be the direct coupling of the FEHM (Zyvoloski et al. 1997) particle tracker used for modeling transport in the UZ with RIP.

Figure 3.10-1 shows the primary components of the RIP model and the information feeds into these components. The primary components are highlighted in the center of the figure, contained within the dotted outline labeled "Run with RIP." They include:

- The waste package degradation model, a callable external routine (WAPDEG) (CRWMS M&O 1998b).

- The waste form degradation model, a combination of callable external routines and functional or stochastic representations directly in RIP.

- The EBS transport model, a series of connected mixing cells.

- The UZ transport model, a callable external routine (FEHM).

- The SZ transport model, a callable external routine (SZ Convolute).

- BDCFs, response surfaces in RIP (functions of climate).

As discussed in Section 1, the primary outputs of the Yucca Mountain process models are described in a series of AMRs. These outputs are input directly (or sometimes with minor postprocessing) into the total system model, illustrated in Figure 3.10-1 by the abstraction or submodel boxes above and beneath the primary RIP component boxes. The AMR number corresponding to the given abstraction (e.g., Seepage Flow Abstraction) or submodel (e.g., UZ Colloid Transport Model) is also listed.

There is not enough room on the figure to list the numerous input parameters required by the TSPA model, only the model or abstraction AMR that produces these input parameters. Therefore, Table 3.10-1 is provided as a complete listing of the input parameters (with associated uncertainty) produced by the AMRs that feed directly into the TSPA model, and which are required to generate dose rate in the biosphere. In effect, Table 3.10-1 is a detailed summary of Sections 3.1 to 3.9 of this chapter. It represents the link between the process models described in the PMRs (and developed through the AMRs) to the TSPA model.

Table 3.10-1. Attributes and Factors Affecting Expected Postclosure Performance and their Corresponding TSPA-SR AMR and the Input Parameters to the TSPA Model Required from Each AMR

Key Attributes of System	Factors	Derived from Analyses/ Model Report	Analyses/Model Report Title	Input Parameters to TSPA-SR
Water Contacting Waste Package	Climate	U0005	Climate Model Abstraction	• Climate States • Timing and Sequence
	Infiltration	U0095	Infiltration Uncertainty Abstraction	• Probabilities for Different Infiltration Scenarios
	UZ Flow Above Repository	U0125	UZ Flow Fields Abstraction	• Flow Fields for Different Infiltration Scenarios and Climate States
	Seepage into Drifts	U0120	Drift Seepage and Coupled Process Abstraction	• Seepage Flux and Seepage Fraction as a Function of Percolation Flux
		E0130	Near-Field Thermodynamic Environment Abstraction	• Percolation Flux–f (Region, Time, Climate)
	Coupled Processes–Effects on UZ Flow	U0115	UZ Coupled Process Flow Field Abstraction	• Flow Fields Affected By TH
	Coupled Processes–Effects on Seepage	U0120	Drift Seepage and Coupled Process Abstraction	• Seepage Flux and Seepage Fraction as a Function of Percolation Flux
		E0130	Near-Field Thermodynamic Environment Abstraction	• Percolation Flux–f (Multiple Locations, Waste Type, Time, Climate)
	Environment on Drip Shield	E0130	Near-Field Thermodynamic Environment Abstraction	• Temperature and Relative Humidity on the Drip Shield Surface–f (Multiple Locations, Waste Type, Time, Climate)
		E0010	EBS Physical Chemical Environment Abstraction	• pH–f (Region, Time) • Fluoride–f (Region, Time) • Chloride–f (Region, Time) • Sulphate–f (Region, Time) • Nitrate–f (Region, Time) • Total Dissolved Carbonate [CO3]T–f (Region, Time) • Oxygen Fugacity–f (Region, Time) • CO2–f (Region Time)
		E0025	EBS Water Distribution and Removal Abstraction	• Seepage Flux Through the Drip Shield • Fraction of Drip Shield Surface That is Wet

Table 3.10-1. Attributes and Factors Affecting Expected Postclosure Performance and their Corresponding TSPA-SR AMR and the Input Parameters to the TSPA Model Required from Each AMR (Continued)

Key Attributes of System	Factors	Derived from Analyses/ Model Report	Analyses/Model Report Title	Input Parameters to TSPA-SR
Water Contacting Waste Package	Performance of Drip Shield	W0075	Juvenile Failures	• Probability of the Occurrence of Material and Manufacturing Defect Flaws • Size of Material and Manufacturing Defect Flaws
		W0125	Abstraction of Model for Mechanical Damage and Failure of Drip Shield and Waste Package by Rockfall	• Time and Size of Rockfall Induced by Seismic Activity • Damage (Cold Work Stress and Through-Wall Crack) as a Function of Rock Size and Remaining Thickness
		W0005	Abstraction of Models for General Corrosion of Drip Shield and Waste Package Outer Barrier	• Threshold for General Corrosion Initiation • General Corrosion Rate Under Drip and No-Drip Conditions • Penetration Opening Size (or Patch Size) by General Corrosion
		W0040	Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier	• Pitting Corrosion Initiation Threshold • Pit Density Distribution • Pitting Corrosion Rate • Effect of Material and Manufacturing Defects on Initiation and Penetration Rate of Pitting Corrosion • Effect of Rockfall Damage on Initiation and Penetration Rate of Pitting Corrosion • Pit Penetration Opening Size Distribution

Table 3.10-1. Attributes and Factors Affecting Expected Postclosure Performance and their Corresponding TSPA-SR AMR and the Input Parameters to the TSPA Model Required from Each AMR (Continued)

Key Attributes of System	Factors	Derived from Analyses/ Model Report	Analyses/Model Report Title	Input Parameters to TSPA-SR
Water Contacting Waste Package	Performance of Drip Shield (cont.)	W0040	Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier	• Crevice Corrosion Initiation Threshold • Probability (or Area) of Crevice Formation on Drip Shield • Crevice Corrosion Rate • Effect of Material and Manufacturing Defects on Initiation and Penetration Rate of Crevice Corrosion • Effect of Rockfall Damage on Initiation and Penetration Rate of Crevice Corrosion • Crevice Penetration Opening Size Distribution
		W0045	Abstraction of Models for SCC of Drip Shield and Waste Package Outer Barrier and HIC of Drip Shield	• SCC Initiation Threshold • Crack Density Distribution • SCC Crack Growth Rate • Effect of Material and Manufacturing Defects on Initiation and Crack Growth Rate of SCC • Effect of Rockfall Damage on Initiation and Crack Growth Rate of SCC • Crack Penetration Opening Size Distribution by SCC
				• HIC Initiation Threshold • Crack Density Distribution • HIC Crack Growth Rate • Effect Material and Manufacturing Defects on Initiation and Crack Growth Rate of HIC • Effect of Rockfall Damage on Initiation and Crack Growth Rate of HIC • Crack Penetration Opening Size Distribution by HIC
		W0030	Failures Due to Mechanical Degradation	• Drip Shield Failure Due to Rockfall

Table 3.10-1. Attributes and Factors Affecting Expected Postclosure Performance and their Corresponding TSPA-SR AMR and the Input Parameters to the TSPA Model Required from Each AMR (Continued)

Key Attributes of System	Factors	Derived from Analyses/ Model Report	Analyses/Model Report Title	Input Parameters to TSPA-SR
Waste Package Lifetime	Environment on Waste Package	E0010	EBS Physical Chemical Environment Abstraction	• pH–f (Region, Time) • Fluoride–f (Region, Time) • Chloride–f (Region, Time) • Sulphate–f (Region, Time) • Nitrate–f (Region, Time) • Total Dissolved Carbonate [CO3]T–f (Region, Time) • Oxygen Fugacity–f (Region, Time) • CO_2–f (Region, Time)
		E0130	Near-Field Thermodynamic Environment Abstraction	• Average Temperature on Waste Package Surface–f (Waste Type, Region, Time, Climate) • Temperature and Relative Humidity on Waste Package Surface–f (Multiple Locations, Waste Type, Time, Climate)
		E0025	EBS Water Distribution and Removal Abstraction	• Seepage Flux Through Waste Package • Fraction of Waste Package Surface that is Wet
	Performance of Waste Package Barrier	W0050	WAPDEG Analysis	• Waste Package Geometry • Thickness of the Different Barriers
		W0020	Aging and Phase Stability of Waste Package Outer Barrier	• Phase Stability and Thermal Aging of Alloy 22 Outer Barrier–Volume Fraction of Secondary Phase as a Function of Time and Temperature
		W0125	Abstraction of Model for Mechanical Damage and Failure of Drip Shield and Waste Package by Rockfall	• Time and Size of Rockfall Induced by Seismic Activity • Damage (Cold Work Stress and Through-Wall Crack) as a Function of Rock Size and Remaining Thickness

Table 3.10-1. Attributes and Factors Affecting Expected Postclosure Performance and their Corresponding TSPA-SR AMR and the Input Parameters to the TSPA Model Required from Each AMR (Continued)

Key Attributes of System	Factors	Derived from Analyses/ Model Report	Analyses/Model Report Title	Input Parameters to TSPA-SR
Waste Package Lifetime	Performance of Waste Package Barrier (cont.)	W0005	Abstraction of Models for General Corrosion of Drip Shield and Waste Package Outer Barrier	• Threshold for General Corrosion Initiation Under Drip (After Drip Shield Failure) and No-Drip Conditions • General Corrosion Rate Under Drip (After Drip Shield Failure) and No-Drip Conditions • Penetration Opening Size (or Patch Size) by General Corrosion
		W0040	Abstraction of Models for Pitting and Crevice Corrosion of Drip Shield and Waste Package Outer Barrier	• Pitting Corrosion Initiation Threshold • Pit Density Distribution • Pitting Corrosion Rate • Effect of Material and Manufacturing Defects on Initiation and Penetration Rate of Pitting Corrosion • Effect of Phase Stability and Thermal Aging on Initiation and Penetration Rate of Pitting Corrosion • Effect of Rockfall Damage on Initiation and Penetration Rate of Pitting Corrosion • Pit Penetration Opening Size Distribution
				• Crevice Corrosion Initiation Threshold • Probability (or Area) of Crevice Formation • Crevice Corrosion Rate • Effect of Material and Manufacturing Defects on Initiation and Penetration Rate of Crevice Corrosion • Effect of Phase Stability and Thermal Aging on Initiation and Penetration Rate of Crevice Corrosion • Effect of Rockfall Damage on Initiation and Rate of Crevice Corrosion • Crevice Penetration Opening Size Distribution

Table 3.10-1. Attributes and Factors Affecting Expected Postclosure Performance and their Corresponding TSPA-SR AMR and the Input Parameters to the TSPA Model Required from Each AMR (Continued)

Key Attributes of System	Factors	Derived from Analyses/ Model Report	Analyses/Model Report Title	Input Parameters to TSPA-SR
Waste Package Lifetime	Performance of Waste Package Barrier (cont.)	W0045	Abstraction of Models for SCC of Drip Shield and Waste Package Outer Barrier and HIC of Drip Shield	• SCC Initiation Threshold • Crack Density Distribution • SCC Crack Growth Rate • Effect of Material and Manufacturing Defects on Initiation and Crack Growth Rate of SCC • Effect of Phase Stability and Thermal Aging on Initiation and Crack Growth Rate of SCC • Effect of Rockfall Damage on Initiation and Crack Growth Rate of SCC • Crack Penetration Opening Size Distribution by SCC
		W0075	Juvenile Failures	• Probability of the Occurrence of Material and Manufacturing Defect Flaws • Size of Material and Manufacturing Defect Flaws
		W0120	Abstraction of Models for Stainless Steel Structural Material Degradation	• Threshold for General Corrosion Initiation Under Drip (After Drip Shield Failure) and No-Drip Conditions (Underneath the Breached Outer Barrier) • General Corrosion Rate Under Drip (After Drip Shield Failure) and No-Drip Conditions (Underneath the Breached Outer Barrier) • Penetration Opening Size (or Patch Size) by General Corrosion
				• Pitting Corrosion Initiation Threshold (Underneath the Breached Outer Barrier) • Pit Density Distribution • Pitting Corrosion Rate (Underneath the Breached Outer Barrier) • Effect of Material and Manufacturing Defects on Initiation and Penetration Rate of Pitting Corrosion • Pit Penetration Opening Size Distribution

Table 3.10-1. Attributes and Factors Affecting Expected Postclosure Performance and their Corresponding TSPA-SR AMR and the Input Parameters to the TSPA Model Required from Each AMR (Continued)

Key Attributes of System	Factors	Derived from Analyses/ Model Report	Analyses/Model Report Title	Input Parameters to TSPA-SR
Waste Package Lifetime	Performance Of Waste Package Barrier (cont.)	W0120	Abstraction of Models for Stainless Steel Structural Material Degradation	• Crevice Corrosion Initiation Threshold (Underneath the Breached Outer Barrier) • Probability (or Area) of Crevice Formation • Crevice Corrosion Rate (Underneath the Breached Outer Barrier) • Effect of Material and Manufacturing Defects on Initiation and Penetration Rate of Crevice Corrosion • Crevice Penetration Opening Size Distribution
				• SCC Initiation Threshold (Underneath the Breached Outer Barrier) • Crack Density Distribution • SCC Crack Growth Rate (Underneath the Breached Outer Barrier) • Effect of Material and Manufacturing Defects on Initiation and Crack Growth Rate of SCC • Crack Penetration Opening Size Distribution by SCC
Radionuclide Mobilization and Release from the EBS	Environment Within Waste Package	F0170	In-Package Chemistry Abstraction	• pH–f (Region, Time) • Total Dissolved Carbonate $[CO_3]_T$–f (Region, Time) • Oxygen Fugacity–f (Region, Time) • $SiO_{2\,(aq)}$–f (Region, Time) • Ionic Strength–f (Region, Time)
		F0175	In-Waste Package Source-Term Abstraction	• Volume of Water in the Waste Package/Waste Form Cell
		F0135	In-Waste Package Temperature History	• Function for Calculating Waste Form Temperature Based on Waste Package Surface Temperature
	CSNF Waste Form Performance	F0015	Inventory Abstraction	• Number of Packages • Zircaloy-Clad Fuel • Stainless Steel-Clad Fuel • Inventory Per Package

Table 3.10-1. Attributes and Factors Affecting Expected Postclosure Performance and their Corresponding TSPA-SR AMR and the Input Parameters to the TSPA Model Required from Each AMR (Continued)

Key Attributes of System	Factors	Derived from Analyses/ Model Report	Analyses/Model Report Title	Input Parameters to TSPA-SR
Radionuclide Mobilization and Release from the EBS	CSNF Waste Form Performance	F0155	Cladding Degradation Abstraction	• Fraction of Surface Area of Zircaloy-Clad CSNF Exposed as a Function of Time
		F0055	CSNF Degradation Model	• CSNF Intrinsic Dissolution Rate Equation • Specific Surface Area
	DSNF, Navy fuel, Plutonium Disposition Waste Form Performance	F0015	Inventory Abstraction	• Number of Packages • Inventory per Package
		F0065	Other Waste Form Degradation Abstraction	• Appropriate Dissolution Rate Equation • Specific Surface Area
	HLW Glass Waste Form Performance	F0015	Inventory Abstraction	• Number of Packages • Inventory per Package
		F0060	HLW Glass Degradation	• HLW Intrinsic Dissolution Rate Equation • Specific Surface Area
	Solubility Limits of Dissolved Radionuclides	F0095	Dissolved Concentration Limits Abstraction	• Concentration Limits (Solubilities) for all Isotopes Included in TSPA
	Colloid Associated Radionuclide Concentrations	F0115	Colloid Source Term Abstraction	• Types of Waste Form Colloids • Concentration of Colloids • K_d and/or K_c for Various Colloid Types • Fraction of Inventory that Travels as Irreversibly Attached onto Colloids
	In-Package Radionuclide Transport	E0095	EBS Radionuclide Transport Abstraction	• Porosity of Corrosion Products–f (Time) • Saturation of Corrosion Products–f (Time) • Evaporation–f (Temperature, Relative Humidity, Composition)
	Transport Through Invert	E0130	Near-Field Thermodynamic Environment Abstraction	• Thermally Perturbed Saturation in the Invert–f (Waste Type, Region, Time, Climate)
		E0095	EBS Radionuclide Transport Abstraction	• Invert Geometry • Porosity of the Invert • Relative Permeability of the Invert as a Function of the Saturation • Diffusion Coefficient

Table 3.10-1. Attributes and Factors Affecting Expected Postclosure Performance and their Corresponding TSPA-SR AMR and the Input Parameters to the TSPA Model Required from Each AMR (Continued)

Key Attributes of System	Factors	Derived from Analyses/ Model Report	Analyses/Model Report Title	Input Parameters to TSPA-SR
Radionuclide Mobilization and Release from the EBS (cont.)	Transport Through Invert	E0025	EBS Water Distribution and Removal Abstraction	• Volumetric Flux Through the Invert–f (Climate, Time) • Saturation in the Invert After Thermal Pulse–f (Time)
Transport Away from the EBS	Advective Pathways in the UZ	U0065	UZ Transport Particle Tracking Abstraction	• FEHM Particle Tracking Model Coupled to RIP
		U0100	UZ/SZ Transport Properties	• Transport Parameters • Fracture Aperture in Different Units • Dispersivity of Fractures • Dispersivity of Matrix
		U0125	UZ Flow Fields Abstraction	• Flow Fields for Different Infiltration Scenarios and Climate States (FEHM Input Files for the Particle Tracking Model
	Retardation of Radionuclide Migration in the UZ	U0100	UZ/SZ Transport Properties	• K_d for all Isotopes Included in TSPA • Diffusion Coefficients–f (Isotopes, Units)
	Colloid Facilitated Transport in the UZ	U0070	UZ Colloid Transport Model	• K_c and/or Kinetic Colloid Parameters for Plutonium and Americium • Colloid Filtration Factor
	Coupled Processes–Effects on UZ Transport	U0100	UZ/SZ Transport Properties	• K_ds–f (Isotopes, Rock Type)
	Advective Pathways in the SZ	S0055	SZ Flow and Transport Model Abstraction	• Breakthrough Curves–f (Radionuclide, Region) • Input Parameters for Convolution Code • Climate Change Flux Multiplication Factor
		S0050	SZ Flow and Transport Stochastic Parameters	• Flow Fields for SZ Flux Uncertainty • Transport Parameters – Effective Porosity for Porous Media Units – Dispersivity (Longitudinal, Horizontal Transverse, Vertical Transverse) • Fraction of Path Containing Alluvium

Table 3.10-1. Attributes and Factors Affecting Expected Postclosure Performance and their Corresponding TSPA-SR AMR and the Input Parameters to the TSPA Model Required from Each AMR (Continued)

Key Attributes of System	Factors	Derived from Analyses/ Model Report	Analyses/Model Report Title	Input Parameters to TSPA-SR
Transport Away from the EBS (cont.)	Retardation of Radionuclide Migration in the SZ	S0050	SZ Flow and Transport Stochastic Parameters	• K_d for all Isotopes Included in TSPA • Matrix Porosity • Flowing Interval Spacing • Effective Diffusion Coefficient • Fracture Porosity • Bulk Density
	Colloid Facilitated Transport in the SZ			• K_c and/or Kinetic Parameters for Plutonium Desorption • Colloid Filtration Factor
	Dilution of Radionuclide Concentrations in the UZ & SZ	B0015	Water Usage	• Annual Groundwater Usage
	Biosphere Transport and Uptake	B0075	Biosphere Dose Conversion Factors	• Biosphere Dose Conversion Factor–f (Radionuclide, Irrigation Time)
Effects of Disruptive Events	Factors for Igneous Activity Scenarios	T0015	Framework for Igneous Activity	• Probability of Igneous Activity
		T0070	Consequence Analysis of Direct Release	• Concentrations at 20 km from Calculations Using ASHPLUME
		B0055	Disruptive Events BDCF	• Biosphere Dose Conversion Factors–f (Radionuclide)
		B0005	Radionuclide Removal from Soil	• Factor to Account for Radionuclide Removal from Soil
	Factors for Seismic Activity Scenarios	T0075	Framework for Seismicity/Structural Deformation	• Probability of Seismicity/Structural Deformation
		T0105	RIP Source/ Seismic Rockfall	• Time and Waste Package Wall Thickness • Rock Size
		T0110	Consequence Analysis Result	• Performance Assessment Consequences of Rockfall, Fault Displacement, and Hydrologic Changes that Could Result from Seismic Activity

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4. TOTAL SYSTEM PERFORMANCE ASSESSMENT ANALYSES

The information presented in this section focuses on the analyses to be conducted for the TSPA SR. The TSPA-SR will present an evaluation of total system performance against the DOE's siting guidelines at 10 CFR 963. 10 CFR 963 is expected to invoke the environmental standards specified by the EPA 40 CFR 197 and the applicable implementing regulations set forth by the NRC proposed 10 CFR 63 (64 FR 8640). Until 10 CFR 963 is promulgated, TSPA-SR will be guided by available regulatory information from the proposed 10 CFR 63 (64 FR 8640). The section describes the TSPA analyses to be conducted to address the regulatory requirements of proposed 10 CFR 63.113 and 10 CFR 63.114 (64 FR 8640). The analyses will be conducted primarily for a 10,000-year time period, consistent with the requirements of proposed 10 CFR 63 (64 FR 8640). Additional analyses supporting the Final EIS will simulate repository performance for longer time periods. With respect to the structure of the TSPA-SR, there are seven major components:

- **Uncertainty and Sensitivity Analysis**–Techniques to (1) propagate uncertainties in model parameters, conceptual models, and future system states, and (2) identify the parameters and processes that are most important to overall system performance.
- **TSPA for the Nominal Scenario**–A compliance evaluation for the nominal scenario consisting of all expected FEPs representing the natural evolution of the repository system.
- **TSPA for the Disruptive Scenarios**–A compliance evaluation for disruptive scenarios considering potentially disruptive FEPs such as igneous activity, but excluding human intrusion.
- **Combination of TSPA Results for Nominal and Disruptive Scenarios**–A compliance evaluation for the overall system developed by probability weighting of the expected value of the dose rates for the nominal and disruptive scenarios.
- **Sensitivity Studies for the Reference Design**–Sensitivity studies conducted for the SR reference design to evaluate design enhancements and alternative design options that may improve overall system performance and reduce the impact of uncertainties.
- **Multiple Barrier Analysis**–Calculational techniques designed to give insight to performance contributions of individual barriers and barrier components.
- **Analysis of Human Intrusion Scenario**–TSPA of a stylized scenario of inadvertent human intrusion through the repository for the purpose of determining the resiliency of the repository system.

These methodology components are described in Sections 4.1 through 4.7.

4.1 TREATMENT OF UNCERTAINTY IN TOTAL SYSTEM PERFORMANCE ASSESSMENT ANALYSES

4.1.1 Uncertainty and its Treatment in the Performance Assessment Process

The assessment of long-term performance for the potential geologic repository at Yucca Mountain involves modeling various coupled thermal, mechanical, geochemical, and/or hydrologic processes taking place within the engineered and natural barriers over extended periods of time, while taking into account uncertainties and their propagation to calculational results. The inherent complexity of these integrated assessments of total system performance also is compounded by various types of uncertainties that may be categorized as:

- **Parameter Uncertainty**–Definitive values for relevant parameters, as well as descriptive measures of their spatial and temporal variability, are difficult to obtain due to limited characterization of the natural system.
- **Conceptual Model Uncertainty**–Alternative process models for various components of the disposal system may be equally likely or defensible because of incomplete understanding, limited information or paucity of data.
- **Scenario Uncertainty**–The future evolution of the geologic environment surrounding the disposal facility is unpredictable.

Here the term uncertainty is used to include stochastic and subjective uncertainty (Helton 1993). Stochastic uncertainty, or variability, arises from differences attributable to geologic heterogeneity. Subjective uncertainty arises from ignorance or imperfect knowledge about processes and/or parameters. The cumulative effect of these uncertainties is that the performance measure of interest (i.e., dose to the average member of the critical group) cannot be estimated exactly. This poses interesting challenges with regard to quantifying and communicating the risks associated with the siting and operation of the disposal facility to the regulators and the general public. Two general approaches (deterministic and probabilistic) have been advocated for the treatment of uncertainty in the performance assessment of geologic disposal systems.

In the deterministic approach, one starts with a reference scenario, a set of reference conceptual models, and a corresponding set of reference parameter sets. The reference scenario describes the performance of the system when all barriers perform according to their respective design criteria (e.g., engineered barriers) or as postulated (e.g., natural barriers). Alternative scenarios are used to describe the failure of individual components, while a "robust" scenario is used to represent pessimistic treatment of uncertainties. Similarly, alternative conceptual models and parameter sets are used to characterize the various sources of conceptual model and parameter uncertainties. The idea is to determine if, given the most pessimistic combination of scenarios (e.g., conceptual models and parameters), the disposal system offers an acceptable margin of safety to humans and the environment from any radionuclide release. The robust assessment approach has been used by the Swiss radioactive waste agency, National Cooperative for the Disposal of Radioactive Waste (Switzerland) (NAGRA) in the Kristallin-I safety assessment (Smith 1994).

The alternative to the deterministic approach is the probabilistic approach wherein the uncertainties in model inputs (parameters) are propagated using statistical methods to produce corresponding uncertainties in model outputs (predictions). Uncertain future events and parameter values are described in a probabilistic framework, from which multiple realizations of future states and model inputs are sampled, and model outputs are computed. The spread in these model outcomes quantifies the uncertainty in the predicted behavior of the system. Benefits of such probabilistic modeling include (1) quantifying uncertainty (i.e., obtaining the full range of possible outcomes and the likelihood of each outcome) for the performance measure of interest, and (2) analyzing the relationship between the uncertain inputs and the uncertain outputs provide insight into the most important parameters.

Several probabilistic performance assessments have been carried out within the U.S. radioactive waste disposal program. These include a series of performance assessment studies for the disposal of transuranic waste at the WIPP (DOE 1996, Chapter 6; Helton et al. 1998), as well as a series of calculations performed for the disposal of HLW at Yucca Mountain by the DOE (Barnard et al. 1992; Wilson et al. 1994; CRWMS M&O 1994; 1995; 1998a, Chapters 1 through 11) and the NRC (NRC 1992; 1995a).

4.1.2 Probabilistic Framework for Uncertainty Propagation

There are two key features of the recently proposed NRC regulation for the potential Yucca Mountain repository. The first is that probabilistic weighting of the consequences of the various uncertain events (i.e., different scenarios) is required. The second is that from the probabilistic calculations, only the expected (i.e., average or mean) value is to be highlighted and used for demonstration of compliance. This is in contrast to the focus on the complementary cumulative distribution function (CCDF), i.e., a graph of exceedance probability versus performance measure, used in previous TSPAs (e.g., CRWMS M&O 1998a, Chapter 11, Section 11.4.1).

In general, the problem of uncertainty propagation in TSPA may be decoupled by separating the aspects of scenario uncertainty from the parametric or conceptual model uncertainty. The process of screening scenarios and assigning a probability of occurrence for each scenario was discussed in Section 2.2. As in previous TSPAs (e.g., CRWMS M&O 1998a, Chapter 11, Section 11.4.1) the process of quantifying the impacts of parameter uncertainty for any given scenario will require a Monte Carlo simulation methodology, which offers the greatest flexibility for uncertainty propagation using complex, nonlinear TSPA models.

For a given scenario, the TSPA model will take the form:

$$D = D(\mathbf{X}_u, \mathbf{X}_c; t) \qquad \text{(Eq. 4.1-1)}$$

where D is the dose rate to a receptor at some prescribed compliance point, $\mathbf{X}_u$ denotes a vector of uncertain parameters ($\mathbf{X}_u = X_{u1}, X_{u2}, \ldots X_{uN}$) numbering N, $\mathbf{X}_c$ denotes a vector of constants and/or fixed parameters ($\mathbf{X}_c = X_{c1}, X_{c2}, \ldots X_{cM}$) numbering M, and t is time. The uncertain parameters are characterized using a cumulative distribution function (CDF) defined as:

$$F(X_{ui}) = P(X_{ui} < x_{ui}); \quad i=1, N \qquad \text{(Eq. 4.1-2)}$$

where i is an index for uncertain variables, and $F(X_{ui})$ denotes the cumulative probability that the variable X_{ui} will have any value less than or equal to X_{ui}. In some cases, the definitions of these distributions are accompanied by specifications of correlations that further define the relations between the uncertain variables X_{ui}.

As noted earlier, the uncertainty in the input variables, X_{ui}, leads to a corresponding uncertainty in the prediction of dose rates. For any one scenario this uncertainty can be summarized by the mean dose, $\overline{D}$. Regulations require that mean doses for each scenario be weighted by scenario probabilities and combined to yield the expected annual dose (See Section 4.4). The steps in the probabilistic performance assessment methodology are briefly described below.

Selecting Imprecisely Known Model Input Parameters to be Sampled–A typical TSPA model may consist of about 1,000 variables, many of which are uncertain. However, specifying distributions for all such variables in Monte Carlo simulation is not necessary or cost-effective. In recent guidance on the use of Monte Carlo analysis for health risk assessments (EPA 1997), the EPA suggested restricting the use of probabilistic assessment to important parameters and pathways based on a systematic preliminary sensitivity analysis. Another motivation for seeking such simplification is the fact that complex total system models often are only found to be weakly sensitive to many of the variables.

Methods that will be used in TSPA-SR to select which uncertain inputs will be carried forward for a full probabilistic analysis include:

- Professional judgment
- Deterministic "one-off" sensitivity analysis using 5th and 95th percentile values
- Sensitivity information obtained from detailed process model runs.

These methods will help identify the key sensitivities, which can then be modeled as uncertainties in the subsequent probabilistic performance assessment calculations.

Constructing Probability Distribution Functions for each of These Parameters–The probabilistic framework employed in Monte Carlo simulations requires that the uncertainty in model inputs be quantified using probability distributions. Previous TSPAs (e.g., CRWMS M&O 1998a, Chapters 1 through 11) have used a variety of sources for generating such information:

- Actual measurements (e.g., porosity of various hydrogeologic units)
- Expert elicitation (e.g., dilution factors in the SZ)
- Process model output (e.g., fraction of waste packages exposed to seeps)

TSPA-SR will continue to use these approaches for generating the required probability distributions. To this end, a guiding principle will be the acceptance Criteria T2, established by the NRC, as outlined in the TSPA&I:

> "Parameter values, assumed ranges, probability distributions, and/or bounding assumption values used in the TSPA are technically defensible and reasonably account for uncertainties and variabilities" (NRC 1998a, p. 10).

Specific guidance on the acceptance criteria related to each of the KESAs is given in the TSPA&I (NRC 1998a).

Generating a Sample Set by Selecting a Parameter Value from each Distribution–The next step in the Monte Carlo process requires generating a number of equiprobable input data sets which consist of parameter values randomly sampled from the prescribed range and distributions. The conventional sampling approach employs purely random sampling, in which each sample element is selected independently of the preceding sampling elements. Thus, sampling is undertaken with replacement and there is no assurance that all regions of the uncertain parameter space have been adequately sampled (especially those believed to be important but with low probabilities of occurrences). Improved sampling can be achieved with Latin hypercube sampling (LHS), where full coverage of the range of each variable is ensured by dividing the range into several intervals of equal probability and selecting a value at random from each interval without replacement (Helton 1993). The LHS methodology is typically employed in conjunction with the restricted pairing technique (Iman and Conover 1982) to ensure that the sampling algorithm imposes the desired correlation structure while eliminating spurious correlation due to the finite size of the sample.

With respect to the performance assessment model described in Equation 4.1-1, the LHS algorithm generates sample sets of the form

$$\{\mathbf{X}_u\}_j = \{X_{u1}, X_{u2}, \ldots X_{un}\}_j \; ; \; j=1, \mathrm{N} \qquad \text{(Eq. 4.1-3)}$$

where j is an index for the LHS sampling. The number of LHS samples required for each situation, N, is problem specific and performance measure dependent.

Calculating Outcomes for the Sample Set and Aggregating Results for all Samples–In this step of the Monte Carlo methodology, the model describing the behavior of the system for the scenario of interest is evaluated for each of the randomly generated parameter sets. This is a simple operation consisting of multiple model calls, where the outcome D_j corresponding to each LHS sample set $\{\mathbf{X}_u\}_j$ is computed. Once all of the required model runs (one for each LHS sample) have been completed, the overall uncertainty in the predicted outcome can be characterized by: (1) summary statistics such as the mean and standard deviation, and (2) the entire distribution, presented either as dose time histories for each realization, or as the CDF or its complement, the CCDF of peak dose independent of time. At any time, the mean and standard deviation of the dose rate are computed as:

$$\overline{D} = \frac{1}{N} \sum_{j=1}^{N} D_j \qquad \text{(Eq. 4.1-4)}$$

$$\sigma[D] = \sqrt{\frac{1}{N} \sum_{j=1}^{N} \{D_j - \overline{D}\}^2} \qquad \text{(Eq. 4.1-5)}$$

As noted earlier, the proposed 10 CFR 63 (64 FR 8640) uses the expected value of the dose as the performance objective. Furthermore, an indication of the uncertainty in the calculated peak dose (likelihood versus individual values of peak dose) is provided by the CCDF.

4.1.3 Deterministic Sensitivity Analysis

A deterministic sensitivity analysis is built around the deterministic base case. which is constructed by choosing some particular value (e.g., mean, median) for each of the TSPA model parameters. The utility of this scenario is not in demonstrating compliance, but in providing insights as to how the various model inputs influence the model outcome.

The objective of the deterministic sensitivity analysis is to determine how changes in particular input parameters affects the model output when all other parameters are held fixed at their initial values. To this end, two measures are used for determining the sensitivities. The first measure is a normalized form of the classical sensitivity coefficient, which is defined as:

$$S_{\mathrm{det},i} = \frac{\partial y}{\partial x_i} \bullet \frac{x_i}{y} = \frac{\partial(\ln y)}{\partial(\ln x_i)} \qquad \text{(Eq. 4.1-6)}$$

where $S_{\mathrm{det},i}$ denotes the normalized deterministic sensitivity coefficient for the i-th parameter x_i, and y is the model outcome. This measure indicates the percentage change in the model outcome (y) corresponding to a one percent change in the variable of interest (x_i). Thus, $S_{\mathrm{det},i}$ can be thought of as a normalized (dimensionless) local gradient in the functional parameter space.

The second measure uses the difference between the model outcomes corresponding to reasonable minimum and maximum values (e.g., 5th and 95th percentiles) of the input parameter of interest to construct a tornado chart. As demonstrated in Figure 4.1-1, the tornado chart shows the range in model predictions corresponding to comparable changes in the underlying model inputs (e.g., $\pm 2\sigma$, Figure 4.1-1). The tornado chart is a useful visual tool for identifying the variables that have the greatest influence on the model outcome. Such information is valuable in screening uncertain inputs to determine which ones will be carried forward for a full probabilistic analysis. In addition to the visual representation, an uncertainty index can be defined by taking the ratio of the model outcomes corresponding to the maximum and minimum values of the parameters:

$$U_i = \frac{y(x_i = \max)}{y(x_i = \min)} \qquad \text{(Eq. 4.1-7)}$$

The uncertainty index provides a quantitative version of the tornado chart. The uncertainty index also indicates whether the parameter has a direct or inverse influence on the model outcome depending on whether its value is greater or less than 1.0.

The sensitivity coefficient and the uncertainty index are to be applied at a given point in time, such as the time of peak dose during the compliance period, at 10,000 years, or at any user-defined time. In addition, time history plots of the model runs corresponding to the reasonable minimum and maximum values (e.g., 5th and 95th percentiles) of the input parameters, where the inputs are perturbed one at a time, are useful qualitative indicators of how input parameters influence the model outcome.

4.1.4 Probabilistic Sensitivity Analysis

While deterministic calculations are useful for obtaining insight as to how the TSPA model works and the interrelationship among model components, ultimately the demonstration of compliance relies on probabilistic calculations. To this end, probabilistic sensitivity analyses are useful for examining how the uncertain inputs affect the expected value and the uncertainty in the computed model outcome. A variety of tools will be employed in TSPA-SR for this purpose.

Scatter Plots–Two of the objectives of probabilistic sensitivity analysis are to identify the input variables that dominate the statistical uncertainty in the output, and to quantify the strength of their influence. The simplest tool for such analyses is the scatter plot, which is a plot of sampled numerical values of an uncertain (independent) variable used in the computations (i.e., the input values) versus the calculated results such as peak dose (i.e., the output values). If little or no relationship exists between an independent variable and the model outcome, the scatter plot will resemble a random distribution of points. However, if a notable relationship exists between them, the plotted points will cluster and exhibit a recognizable form. Scatter plots also help reveal threshold phenomena and nonlinearities (or lack thereof) in the input-output relationship. Scatter plots also may be used to examine relationships between pairs of output variables.

Correlation and Regression Analyses–Scatter plots are valuable for identifying a relationship between an input variable and an output variable, but they do not quantify the intensity of that relationship. In performance assessment studies, multiple linear regression modeling commonly is used for this purpose (Helton 1993). Using regression models, it is possible to identify input variables that contribute the most to calculated uncertainty (variance) in the performance measure. The primary technique for regression modeling is stepwise linear regression (in this case, using rank transformations to linearize the problem). In the stepwise approach, a sequence of regression models is constructed starting with a single selected input parameter (usually the parameter that explains the largest amount of variance in the output), and including one additional input variable at each successive step (usually the parameter that explains the next largest amount of variance) until all input variables that explain statistically significant amounts of variance in the output have been included in the model. This approach avoids having to treat all independent uncertain variables simultaneously in a single model.

Two indicators are used to rank the input variables, partial rank correlation coefficient and R^2-loss (where R^2 denotes the coefficient of determination for the regression model). Both of these indicators are calculated during stepwise regression modeling. The partial rank correlation coefficient for a particular input variable measures the correlation between the output and the selected input variable, after the linear influences of the other variables in regression have been eliminated (Helton 1993). The square of a partial rank correlation coefficient can be used to calculate the gain in R^2 of the regression model (expressed as a fraction of the currently unexplained uncertainty) as the selected variable is brought into regression (RamaRao et al. 1998). The second importance indicator used (R^2-loss) represents the loss in R^2 of the current n-variable regression model, if the variable of concern is dropped from the regression model. A large value of R^2-loss (i.e., a large decrease in explanatory power) indicates that the removed variable explained a large proportion of the variance in the output, and therefore, that the variable is an important component of the model.

Probabilistic Sensitivity Coefficients and Distribution Reweighting Methods–As described earlier, the proposed 10 CFR 63 (64 FR 8640) stipulates the use of the expected (i.e.. average) dose to demonstrate compliance, as opposed to previous standards relying on the entire cumulative distribution. Because the expected dose is derived from a complete probability distribution, the sensitivity analysis methods for quantifying the sensitivity of the output variance to the inputs are useful. However, new metrics are required to capture the sensitivity of the output mean to the inputs. In TSPA-SR, it is proposed that a probabilistic version of the normalized deterministic sensitivity coefficient be used for this purpose. The mean sensitivity coefficient measures the percent change in the output mean, corresponding to a one percent change in the mean of the inputs:

$$MSC\ (X_{ui}) = \frac{\partial \overline{D}}{\partial \overline{X}_{ui}} \bullet \frac{\overline{X}_{ui}}{\overline{D}} = \frac{\partial (\ln\ \overline{D})}{\partial (\ln\ \overline{X}_{ui})} \qquad \text{(Eq. 4.1-8)}$$

Here $\overline{D}$ denotes the conditional mean dose rate for a single scenario, and $\overline{X}_{ui}$ denotes the mean of the variable X_{ui}. In general, this is related to the quantity defined in Equation 4.1-6, except that the output mean cannot be obtained simply by using the mean of all the model inputs because of model nonlinearity.

In general, the evaluation of the mean sensitivity coefficient requires an investigation of how the output distribution (i.e., its moments) are altered if selected input distributions are modified by changing their moments. A low sensitivity of the moments of output distribution, such as the mean and the variance, to the input parameter distributions is an indicator of the robustness of the estimates of the performance measures. To study this aspect, replicate Monte Carlo simulations can be performed; but this method becomes impractical for the complex models with a large number of inputs as in the Yucca Mountain modeling studies. Alternative computational schemes, without recourse to additional Monte Carlo realizations, are available for this purpose (e.g., Iman and Conover 1982) and are proposed for use in this study. These methods belong to a class of reweighting schemes, which involve simple post-processing of the inputs and outputs of the Monte Carlo simulations. These numerical methods are particularly suited to the LHS schemes used in the uncertainty modeling studies here.

Consider the impact of a change in the distribution of the input variable, X_{ui}, on the mean of the output distribution, without doing a new Monte Carlo simulation (i.e., using the previously simulated D_i (i=1, N)). Because no new simulations are undertaken, the previously determined equiprobable intervals on each input variable, their upper and lower bounds, and the random location of the observation in this interval are assumed to be unchanged from the case of modified input distribution(s). The original interval, and its bounds, can be transferred onto the new distribution for X_{ui}. The probability that the random observation is in this interval can be found by the area enclosed between the bounds on the probability density function for X_{ui}. Equivalently, the probability can be determined by the difference between the ordinates on the CDF, corresponding to the upper and lower bounds of the interval. The modified probability of the interval, or the observation in this interval, alters the probability of each of the input vectors. Thus, the probability weighted sum of D_i (i=1, N) can be recomputed, taking care to normalize the weights. This method involves re-computing the probabilities of the previously selected input vectors in the context of the revised input distribution(s). Because the mean is computed as a weighted sum of the N values of D, with the weights changing from LHS to the modified distribution case, this method is known as a distribution reweighting method (DRM).

Previous studies have used the DRM primarily to investigate the change in the mean of the output if the underlying distribution is modified (NRC 1980). The methodology needs to be tested to ensure that it provides robust answers for the new sensitivity measures (i.e., mean sensitivity coefficient) proposed here.

Identification of Key Drivers of Risk–It is important to distinguish between two key features of sensitivity analysis as described here: (1) methods that identify those variables which drive performance, and (2) methods that identify those variables that drive the uncertainty in performance. In general, the importance ranking from the two methods will not be identical, because the results from the first set of methods are based on the sensitivity of the model outcome to a given input. The results from the second set of methods are based on the uncertainty in a given parameter as well as the sensitivity of the model outcome to that parameter. This subtle, yet important, distinction often is not appreciated and leads to apparent inconsistencies in ranking importance of input parameters.

Probabilistic sensitivity analyses based on linear regression must be interpreted carefully. A regression based sensitivity analysis will not give an uncertain variable a high importance ranking if it does not produce a relatively wide range of calculated output values. In other words, a parameter will not be assigned a high importance ranking unless it accounts for a large fraction of the variance in the output measure being analyzed. Therefore, the magnitude of peak dose rate may be strongly affected by a certain parameter, but if the range of uncertainty associated with that parameter is relatively small, the parameter may not be found to be important. As an example, neptunium solubility was not found to be an important variable in the TSPA-VA, but because neptunium-237 often dominates the calculated dose rates, it clearly does influence the total peak dose rate. The reason neptunium solubility did not appear as an important variable in the regression based sensitivity analysis for TSPA-VA was largely due to the wide uncertainty ranges associated with seepage fraction and waste package corrosion.

Additional insight into relative importance of various uncertain inputs is obtained using the mean sensitivity coefficient, the normalized deterministic sensitivity coefficient, and the uncertainty index. These coefficients provide information as to how the mean of the output distribution is sensitive to the mean of the uncertain inputs, as well as how the deterministic model outcome changes when the inputs are altered locally or globally. Identification of key drivers of risk requires that these metrics be examined in conjunction with the results from the regression based sensitivity analysis.

4.2 NOMINAL-SCENARIO DOSE ANALYSES

As explained in Section 2.2, the nominal scenario is defined as the scenario containing all of the expected FEPs but none of the D FEPs. The nominal scenario is considered to be most representative of the actual evolution of the repository system. This scenario does not include major disturbances like volcanic intrusions or new faults within the repository, but it does include expected disturbances such as changes in climate and seismicity. The probability of the nominal scenario is computed as one minus the sum of disruptive event probabilities.

The nominal scenario for the TSPA-SR will include propagation of uncertainties in both conceptual models and model parameters. Consequently, calculational output for the nominal scenario will be probabilistic (i.e., statistical distribution of dose rate at 20 km). However, deterministic analyses may be used for illustration, as well as for some types of sensitivity analysis. The method used for probabilistic analysis is Monte Carlo simulation. A consequence model for the system and a set of input parameters for the model (including probability distributions for key uncertain parameters) are required for a Monte Carlo simulation. For TSPA-SR, the consequence to be calculated is the "annual dose to the average member of the critical group," as stated in proposed 10 CFR 63.113(b) (64 FR 8640, pp. 8676 through 8677). The consequence model is the TSPA model described in Section 3.10. The TSPA model for the nominal scenario incorporates key component models that are described in Sections 3.1 through 3.8. Each of these sections includes a general description of the model, its subcomponents, and the assumptions used for the TSPA-SR. The model descriptions contain some details about the cases and parameters that will be used for the TSPA calculations, and, in particular, for the nominal scenario. The key uncertain parameters for each component are also discussed. The calculational result of the probabilistic simulation of the nominal scenario will be a set of *N* time histories of annual dose (*N* is the number of realizations that were specified for the simulation). For the VA, *N* was typically 100, though the effect of using higher *N* was tested (DOE 1998a, Section 4.3.1.2). The number of realizations to be used for TSPA-SR will be determined through a series of calculations. The criterion for choosing the number of realizations is that it must be high enough to provide a stable estimate of the expected annual dose.

A comparison with the dose limit set in proposed 10 CFR 63.113(b) (64 FR 8640, pp. 8676 through 8677) requires calculating the mean annual dose for the nominal scenario and combining it with the mean annual doses for the disruptive scenarios, appropriately weighted by the probability of each scenario (see Section 4.4). However, much can be learned by analyzing the results of the nominal scenario separately as well. A set of 100 (or more) dose histories, together with the sets of input parameters for each history, represents a great deal of information that can be analyzed in a number of different ways. It is of interest to calculate the mean dose history (averaging all calculated doses at each time step and weighting by the probability of the nominal scenario) and to find its maximum value, to show how close the nominal scenario alone is to the dose limit. The uncertainty and sensitivity analyses described in Section 4.1 and the multiple barrier analyses described in Section 4.5 are expected to be applied to the nominal scenario to gain better understanding of the nominal-scenario performance and the role of the TSPA component models.

4.3 DISRUPTIVE SCENARIOS ANALYSES

As described in Section 2.2, a DFEP is a retained FEP that has a probability of less than 1 (but greater than the cutoff of $10^{-4}/10^{4}$ year, set by the NRC). Retained, as used here, implies that the DFEP potentially could have an important impact on performance. The disruptive scenarios are defined by the occurrence of one or more disruptive FEPs and includes all of the EFEPs. It is important to note that scenario, as used here, is equivalent to the term scenario class used by the NRC (1998a).

The total number of scenarios considered in the TSPA will be determined by the combinations of the occurrence and nonoccurrence of the disruptive events identified in the FEP screening process. Three potentially disruptive events are identified in the TSPA-VA (CRWMS M&O 1998a, Chapter 10, Section 10-4, 10-5, and 10-6) resulting in eight scenarios (one nominal scenario and seven disruptive scenarios) (see Figures 2.2-3 and 2.2-4). Quantitative analyses done for the TSPA-VA focused on only three of the disruptive scenarios: igneous activity, seismic activity, and criticality (CRWMS M&O 1998a, Chapter 10). Analyses of the scenarios involving combinations of disruptive events (e.g., the igneous activity and seismic activity scenario) were not included in the VA (DOE 1998a, Section 4), but they will need to be examined in the TSPA-SR if multiple disruptive events are retained for analysis. As described in Section 2.2.3, scenarios formed by the combination of multiple disruptive events will be screened on the basis of probability and consequence before being included in the overall calculation of expected annual dose, described in Section 4.4.

4.3.1 Disruptive Scenario Probability Analysis

Probabilities of disruptive scenarios are based directly on the probabilities determined for the disruptive events that define them. Specifically, the probability of any single scenario is the joint probability (i.e., the multiplicative product) of individual probabilities of occurrence and nonoccurrence of the defining events. For example, if each of three disruptive events were determined to have a probability of occurrence of 0.01 in 10,000 years, the probability of the nominal scenario in which none of the three events occurs is equal to (0.99)(0.99)(0.99) = 0.9703. The probability of a scenario in which one, and only one, of these hypothetical disruptive events occurs would be equal to (0.99)(0.99)(0.01) = 0.0098. The probability of a scenario in which all three of these hypothetical disruptive events occur would be (0.01)(0.01)(0.01) = 0.000001, or 10^{-6}. This probability falls below the $10^{-4}/10^{4}$ year cutoff prescribed by the NRC, and the hypothetical scenario containing all three events would therefore not be included in the quantitative dose analysis. To ensure logical completeness in the summing of scenario probabilities, the probabilities of the remaining seven scenarios in this example would be adjusted appropriately to reflect this exclusion.

FEP screening is, at the present time, incomplete for the TSPA-SR, and the total number of disruptive events that will be used to define disruptive scenarios is unknown. Preliminary work indicates that igneous activity will be treated as a disruptive event. Therefore, an estimate of the probability of igneous activity will be needed for the scenario analysis. The probability of igneous activity at Yucca Mountain is discussed in Section 3.9. The treatment of the other potentially disruptive events considered in the VA (DOE 1998a, Section 4) is being examined through the FEP screening. Definitive statements about the screening decisions for seismic activity and criticality, and for all other FEPs, are not available at the present time.

4.3.2 Disruptive Scenario Consequence Analysis

Models will be developed that allow quantitative analysis of repository performance for each of the retained disruptive scenarios (i.e., those remaining after screening). Models for the disruptive scenarios will be based on process models consistent with available data and other information. Disruptive scenarios will also require the development of some models specific to the event in question (Section 3.9). For example, analysis of the consequences of igneous activity requires development of models and data characterizing the interactions between the waste and a volcanic vent that intersects the repository.

Multiple annual dose histories and the mean annual dose history will be calculated for each disruptive scenario with a probability above the NRC cutoff. This mean annual dose history differs from the expected annual dose required by proposed 10 CFR 63.113(b) (64 FR 8640), in that it is the conditional mean dose that would result if the scenario occurs. As described in Section 4.4, the conditional mean dose for each scenario (both nominal and disruptive) must be weighted by the probability determined for that scenario before the dose histories are summed to construct the expected annual dose. The conditional annual dose histories calculated for individual disruptive scenarios (or the nominal scenario), therefore, have no specific regulatory significance, taken independently. Comparisons with the dose limit set at proposed 10 CFR 63.113(b) (64 FR 8640) should be made using the combined nominal and disruptive scenario analysis results reported in Section 4.4.

4.4 COMBINED NOMINAL AND DISRUPTIVE SCENARIO ANALYSES

As specified in proposed 10 CFR 63.113(c) (64 FR 8640), the TSPA for a compliance demonstration must consider, all expected and FEPs that have not been excluded through a systematic FEPs scenario screening process (see Section 2.2). Specifically, the expected annual dose used for comparison with the 25 mrem/year dose rate limit in the proposed 10 CFR 63.113(b) (64 FR 8640) must be estimated "considering the probability of the occurrence of the events and the uncertainty, or variability, in parameter values used to describe the behavior of the geologic repository" (proposed 10 CFR 63.2 (64 FR 8640)).

In the TSPA&I, Revision 01 (NRC 1998a, Appendix D, pp. D-2 through D-5), the NRC provides definitive guidance on the methodology for combining the probabilistic calculations (for expected annual doses) for the nominal and disruptive scenarios. The approach adopted for the TSPA-SR is consistent with this NRC guidance. More specifically, the probabilistic calculations of the expected annual dose histories for the nominal and disruptive scenarios will be combined through a probability weighting method to produce a quantitative result suitable for comparison with the regulatory limit. This expected annual dose includes the likely performance of the disposal system (the nominal scenario) and the consequences of unlikely events (the disruptive scenarios). The expected annual dose to the average member of the critical group will be based on a TSPA that includes the effects of uncertainty and variability in the input parameter values used to describe the behavior of the system in both nominal and disruptive scenarios. Consistent with the requirements of proposed 10 CFR 63.113(c) (64 FR 8640), the expected annual dose histories exclude the effects of the human intrusion scenario. The expected annual dose history for the inadvertent human intrusion scenario will be evaluated separately (see Section 4.7) through a TSPA for a stylized human intrusion scenario, designed in accordance with NRC requirements and guidance.

4.4.1 Conditional Mean Dose Histories for Nominal and Disruptive Scenarios

Through the probabilistic TSPA, multiple histories of annual dose will be produced for the nominal scenario and each of the retained disruptive scenarios (Sections 4.2 and 4.3). A Monte Carlo simulation technique will be used to incorporate uncertainty and variability in the model input parameters by using different vectors of sampled values for each realization. Therefore, results for each modeled scenario will include a separate dose history for each sampled vector (1 through *n*). Dose histories for each input vector will be combined to display a conditional mean annual dose history for each scenario (Figure 4.4-1). The use of the term conditional indicates that these are the mean doses expected if the chosen scenario conditions were certain to occur. Because the scenario probabilities partition the probability space, the conditional mean dose histories must be weighted by the scenario probabilities and summed to give the overall expected annual dose history.

Information shown in Figure 4.4-1 will be displayed, in some form, for each scenario included in the TSPA-SR. This information will meet the NRC requirement that the expected annual dose consider uncertainty and variability in the input parameters used in the models.

4.4.2 Probability Weighted Mean Dose Histories for Nominal and Disruptive Scenarios

The conditional mean dose histories (Section 4.4.1) are multiplied by the probabilities assigned to each scenario (Section 4.3.1) to generate probability weighted dose histories (Figure 4.4-2). Display of this information will meet the NRC requirement that the expected annual dose consider the probabilities of the occurrence of the events that have been used to construct the scenarios.

4.4.3 Summing the Probability Weighted Mean Dose Histories for Nominal and Disruptive Scenarios

The probability weighted mean dose histories for each scenario (1 through *m* in this example) will be summed to generate the overall expected annual dose history (Figure 4.4-3), as required by proposed 10 CFR 63.113(b) (64 FR 8640). As required by proposed 10 CFR 63.113(c) (64 FR 8640), this expected annual dose history will have been generated in accordance with the requirements of proposed 10 CFR 63.114 and 63.115 (64 FR 8640) and will exclude the effects of human intrusion.

4.5 MULTIPLE BARRIER ANALYSIS

The multiple barrier analysis methodology to be used in the TSPA-SR has two main objectives. The first objective is to quantify the performance contribution of the barriers and barrier components that have the most influence on overall performance. A multiple barrier analysis approach (see Section 4.5.2) will be applied to explicitly identify how the natural and engineered barriers perform. The second objective is to disaggregate the probabilistic TSPA results for the purposes of explaining and interpreting the cause-and-effect relationships and evaluating the propagation of uncertainties.

4.5.1 Purpose

The TSPA-SR will present an evaluation of total system performance against the DOE's siting guidelines at 10 CFR 963. 10 CFR 963 is expected to invoke the environmental standards specified by the EPA 40 CFR 197 and the applicable implementing regulations set forth by the NRC proposed 10 CFR 63 (64 FR 8640). Until 10 CFR 963 is promulgated, TSPA-SR will be guided by available regulatory information from the proposed 10 CFR 63 (64 FR 8640).

The dose limit prescribed in proposed 10 CFR 63 (64 FR 8640) for the Yucca Mountain repository is an all-pathways dose criterion. The proposed regulation stipulates that the expected annual dose shall not exceed 25 mrem TEDE at any time during the 10,000-year compliance period. Furthermore, in keeping with the overall risk informed spirit of the regulations, this total system standard has not been supplemented with explicit criteria for subsystem (i.e., individual barrier) performance, as was the case with 10 CFR 60. The regulations in proposed 10 CFR 63 (64 FR 8640) call for the DOE to describe the capability of important natural and engineered barriers to isolate waste, so that the NRC may find, with reasonable assurance, that the repository system will be able to achieve the overall safety objective over time frames of thousands of years. In addition to the generic requirements stipulating the need for multiple barriers, as described in proposed 10 CFR 63.102(h) and 63.113(a) (64 FR 8640), the other pertinent sections of the regulations addressing multiple barrier performance may be paraphrased as follows:

- Identify EBS and natural environment features considered barriers important to waste isolation (proposed 10 CFR 63.114(h) (64 FR 8640)).

- Describe the capability of these barriers to isolate waste, taking into account uncertainties in characterizing and modeling them (proposed 10 CFR 63.114(i) (64 FR 8640)).

- Provide the technical basis for analyses in support of the above performance regulations (proposed 10 CFR 63.114(j) (64 FR 8640)).

As stated in Section VIII of the Supplementary Information published with the proposed regulations (64 FR 8640), the objective of these requirements is to:

> Provide for a system of multiple barriers and an understanding of the resiliency of the geologic repository provided by the barriers important to waste isolation to ensure defense in depth and increase confidence that the postclosure performance objective will be achieved (64 FR 8640).

4.5.2 Approach

The overall TSPA methodology, as presented earlier in this document, uses scenarios, conceptual models, and parameters as its building blocks. The evaluation of total system performance, and its uncertainty is, therefore, affected by the probabilistic characterization of scenarios, conceptual models, and parameters. As described in Section 4.1, a Monte Carlo simulation approach will be used for translating the uncertainty in the TSPA model inputs into the uncertainty in the TSPA model output. Finally, as stipulated in the regulations, the TSPA results are presented in terms of the expected annual dose.

The multiple barrier analysis will use the same modeling framework as the TSPA, with one major difference. The scenarios, conceptual models, and parameters are aggregated into barriers, which denote physically distinct components of the system. Examples of such barriers include:

- Waste form
- Waste package
- Engineered barriers within the drift

- UZ
- SZ.

Given this reconfiguration of the modeled system in terms of barriers, two approaches are proposed for TSPA-SR to satisfy the regulatory requirement for a multiple barrier analysis. These include (1) pinch point analysis, which addresses the issue of how the barriers work, and (2) neutralization analysis, which addresses the issue of how the overall performance changes as a function of assumed diminished performance credit for a component barrier. Both approaches are expected to be applied in the TSPA-SR where the results will be compared and contrasted.

The pinch point analysis approach is based on the processing of output from TSPA calculations at subsystem boundaries, or pinch points. These are locations where mass or energy is being transferred from one modeling domain (or subsystem or barrier) to another. The pinch point analysis methodology is analogous to the performance allocation methodology described in CRWMS M&O (1996b) and Vallikat et al. (1998).

In the neutralization analysis approach, barriers are neutralized one at a time starting from the base case. The degradation in performance of the neutralized scenario relative to the base case provides an indication of the relative importance of that barrier. A previous application of this methodology to the Yucca Mountain system has been described by CRWMS M&O (1999d). Conceptually, the methodology is also similar to the importance measures proposed by Eisenberg and Sagar (1998).

4.5.3 Pinch Point Analysis

The engineered and natural barriers seek to isolate waste from the environment by attenuating the movement of radionuclides, thus reducing the amount of mass released, and/or by diluting the radionuclides, thus reducing their concentration (and dose). Therefore, two different metrics are proposed to measure the effectiveness of different barriers for waste isolation. The first metric is related to the reduction in mass, and the second metric is related to the reduction in concentration, as the nuclides are transported through various barriers. These barrier effectiveness measures provide an indication of how the contaminants are distributed throughout the system, as well as an understanding of how the barriers are acting together to provide waste isolation.

Metrics Related to Reduction in Mass–Two different versions of this metric are proposed. The first quantifies the absolute mass reduction within each barrier (i.e., how much mass is retained in each barrier as a fraction of the initial inventory). For barrier *j*, and radionuclide *i*, the first barrier effectiveness factor, BEF1, is defined as:

$$\mathrm{BEF1}_i(j) = [\mathrm{M}_{\mathrm{in},i}(j) - \mathrm{M}_{\mathrm{out},i}(j)] \,/\, \mathrm{M}_{\mathrm{initial},i} \qquad \text{(Eq. 4.5-1)}$$

where M_{in} denotes the mass entering the barrier, $\mathrm{M}_{\mathrm{out}}$ denotes the mass exiting the barrier, and $\mathrm{M}_{\mathrm{initial}}$ denotes the initial inventory.

Figure 4.5-1 provides a visual assessment of such a metric for a single nuclide, technetium-99, in an evaluation of the Canadian repository program (Goodwin et al. 1994). Figure 4.5-1 shows how technetium-99 is retained within different barriers and isolated from the biosphere at two different points in time: 10,000 years and 100,000 years.

The deterministic definition given in Equation 4.5-1 can be extended easily for the probabilistic case by using the linearity property of the expectation operator, as follows:

$$\overline{\mathrm{BEF1}_i(j)} = [\overline{\mathrm{M}_{in,i}(j)} - \overline{\mathrm{M}_{out,i}(j)}] / \mathrm{M}_{initial,I} \qquad \text{(Eq. 4.5-2)}$$

where the bar-over symbol denotes expected value (arithmetic mean).

Note that the definition of BEF1 tends to understate the importance of downstream barriers, which receive a small fraction of the initial inventory. Therefore, a second barrier effectiveness factor (BEF2) is proposed to quantify the relative mass reduction in each barrier, as follows:

$$\mathrm{BEF2}_i(j) = [\mathrm{M}_{in,i}(j) - \mathrm{M}_{out,i}(j)] / \mathrm{M}_{in,i}(j) \qquad \text{(Eq. 4.5-3)}$$

where the inflowing mass for the barrier, M_{in}, is used as the normalizing factor as opposed to the initial inventory, as in Equation 4.5-1.

This measure is related to the absolute performance factor for mass release as defined by CRWMS M&O (1996b), as follows:

$$\mathrm{APF}_i(j) = \mathrm{M}_{in,i}(j) / \mathrm{M}_{out,i}(j) = 1 / [1 - \mathrm{BEF2}_i(j)] \qquad \text{(Eq. 4.5-4)}$$

Either Equation 4.5-3 or Equation 4.5-4 can be used to quantify the relative barrier effectiveness in terms of a mass reduction factor. However, the former is preferable (albeit marginally) because it is bounded in the interval [0,1], which facilitates cross comparison of the performance of a multitude of barriers.

In order to extend Equation 4.5-3 for the probabilistic case, note that the expected value of a random variable, *z*, which is the ratio of two random variables, *x* and *y*, is given by:

$$\bar{z} = \overline{x/y} = \bar{x} \cdot \overline{y^{-1}} \qquad \text{(Eq. 4.5-5)}$$

where the bar-over symbol denotes expected value (arithmetic mean) as before, and *x* and *y* are assumed to be uncorrelated. Thus, the probabilistic versions of Equations 4.5-3 and 4.5-4 can be written as:

$$\overline{\mathrm{BEF2}_i(j)} = [\overline{\mathrm{M}_{in,i}(j)} - \overline{\mathrm{M}_{out,i}(j)}] \cdot \overline{\mathrm{M}_{in,i}(j)^{-1}} \qquad \text{(Eq. 4.5-6)}$$

$$\overline{\mathrm{APF}_i(j)} = \overline{\mathrm{M}_{in,i}(j)} \cdot \overline{\mathrm{M}_{out,i}(j)^{-1}} \qquad \text{(Eq. 4.5-7)}$$

Note that the evaluation of these expressions requires that the expected value of the reciprocal (harmonic mean) of one of the quantities be computed, in addition to the expected values (arithmetic mean) of these quantities.

Metrics Related to Reduction in Concentration (Dose)–A third barrier effectiveness factor (BEF3) to quantify the reduction in concentration (dose) within a given barrier is defined, following CRWMS M&O (1996b), as follows:

$$\mathrm{BEF3}_{i}(j) = C_{out,i}(j) \,/\, C_{in,i}(j) \qquad \text{(Eq. 4.5-8)}$$

where C_{out} is the outflowing concentration (dose) and C_{in} is the inflowing concentration (dose) for the radionuclide and barrier combination of interest. Thus, Equation 4.5-8, which is the reciprocal of the absolute performance factor for dose, as defined by CRWMS M&O (1996b), can be used to define relative barrier effectiveness in terms of a concentration (dose) reduction factor.

The extension of this barrier effectiveness factor to the probabilistic case is based on the statistical identity given by Equation 4.5-5, and can be expressed as:

$$\overline{\mathrm{BEF3}_i(j)} = \overline{C_{out,i}(j)} \cdot \overline{C_{in,i}(j)^{-1}} \qquad \text{(Eq. 4.5-9)}$$

4.5.4 Neutralization Analysis

In the neutralization analysis, the fundamental idea is to examine the extent to which performance of the overall system is affected as a function of assumed reductions or neutralizations of barrier performance. As such, this approach gives some insight into the approximate performance contribution of individual barriers and barrier components.

As in the pinch point analysis, the first step in the neutralization approach is the aggregation of scenarios, parameters, and conceptual models into physically distinct components of the waste disposal system, called barriers, such as:

- Waste form
- Waste package
- Engineered barriers within the drift
- UZ
- SZ.

The TSPA model is then evaluated for the base case with all the barriers performing as expected (including their uncertainties). In the next step, each barrier is neutralized one at a time (i.e., the barrier is assumed to be absent and/or performing at very pessimistic levels). The performance of the neutralized system is computed and compared against that of the base case to determine the relative importance of various barriers. If D is the performance of the base case, and $D^*(j)$ is the performance corresponding to the neutralization of the *j*-th barrier, then following Eisenberg and Sagar (1998), a measure of barrier importance can be defined as follows:

$$I_I(j) = D^*(j) \,/\, D \qquad \text{(Eq. 4.5-10)}$$

where I_I is the importance measure. Note that this definition is strictly applicable for deterministic calculations. Its extension for the probabilistic case follows from the statistical identity given in Equation 4.5-5.

4.5.5 Implementation Issues

The two approaches to evaluating multiple barrier performance have been described using equations that are appropriate for steady-state conditions. The time dependence in the actual computation of performance can be readily handled by making the calculations at the time of peak dose (maximum risk) during the compliance period, the selected time slices during the compliance period, or for all time slices at which the TSPA calculations are carried out.

The metrics proposed above for quantifying the effectiveness of individual barriers in a system with multiple barriers rely on the comparison of mass flux across pinch points (i.e., the entry and exit points for a barrier). As such, an examination of these factors provides information regarding the relative importance of various barriers for waste isolation. Metrics have been proposed to take into account both mass reduction and concentration (dose) reduction, because mass is the fundamental quantity that is to be isolated, while concentration is what drives receptor risk. It is likely that the importance ranking of barriers will depend on the metric being used, but that is to be expected for a system as complicated as Yucca Mountain.

The actual implementation of the neutralization merits some discussion. One approach is to assume that the neutralization of the *j*-th barrier implies that the output (e.g., mass, concentration) from the barrier upstream ([*j-1*]-th barrier) is directly passed to the barrier downstream ([*j+1*]-th barrier) without any attenuation or delay. For the engineered barriers, it is easy to conceptualize this situation, which can be readily modeled by physically removing the engineered component in question from the waste isolation system. The situation is not as straightforward with the natural barriers, where the physical removal of a natural barrier is open to interpretation. Therefore, an alternative is to assume that barrier neutralization is not tantamount to total failure of the barrier, but instead that its performance is at some pessimistic level (e.g., the 95th percentile level).

The neutralization analysis provides a simple, easy-to-understand construct that highlights the scenario of extreme barrier unreliability. As such, the methodology is useful for providing an assessment of performance that takes into account uncertainties not easily parameterized in terms of probability distributions. One potential problem with this approach is the issue of nonlinear feedback and/or dependencies among different subsystems, and how to handle this in the modeling of neutralized scenarios.

4.6 SENSITIVITY STUDIES OF THE REFERENCE DESIGN

The TSPA-SR will present an evaluation of total system performance against the DOE's siting guidelines at 10 CFR 963. 10 CFR 963 is expected to invoke the environmental standards specified by the EPA 40 CFR 197 and the applicable implementing regulations set forth by the NRC proposed 10 CFR 63 (64 FR 8640). Until 10 CFR 963 is promulgated, TSPA-SR will be guided by available regulatory information from the proposed 10 CFR 63 (64 FR 8640).

The proposed NRC regulation, proposed 10 CFR 63.21(b)(7) (64 FR 8640), states that for the potential LA, the DOE Safety Analysis Report shall include "a comparative evaluation of alternatives to the major design features that are important to waste isolation, with particular attention to the alternatives that would provide longer containment and isolation of radioactive materials." For the purposes of the SR, however, the TSPA-SR will focus on analyses of further enhancements to the recently selected reference design (CRWMS M&O 1999a). This section describes the reference design for the SR and discusses the enhanced design alternatives that are expected to be evaluated as sensitivity cases in the TSPA-SR.

The SR reference design follows the recommendations in Section 7 of the *License Application Design Selection Report* (CRWMS M&O 1999a). An important attribute of the reference design is that it ensures relatively low thermal effects (i.e., small alteration zone). The waste emplacement area for the reference design would encompass 1,064 acres (see Figure 4.6-1). The waste package design consists of two layers, with an outer layer of corrosion resistant material (Alloy-22) and an inner layer of stainless steel (SS-316L). The thermal loading strategy for the reference design was selected to maintain the fuel cladding temperature below 350°C and to keep the boiling fronts from coalescing in the pillars between drifts (see Figure 4.6-2).

Preventing boiling fronts from coalescing in the pillars ensures that there will be sufficient portions of the pillar that will have temperatures below the boiling point (less than 96°C, the boiling point of water at the potential repository altitude); this will permit water to drain through the pillars when the adjacent rock is above the boiling point of water. These fuel cladding and thermal-hydrology goals can be achieved with an areal mass loading of 60 MTU/acre that includes closely spaced waste packages, line loading, and drift spacing of 81 m. In addition, the reference design includes backfill material and a 2 cm thick titanium (titanium-7) drip shield over the waste package at closure. The backfill would be placed over the continuous drip shield, after it had been installed over the waste packages but prior to closure. Blending of spent fuel waste would reduce the maximum waste package heat output to within 20 percent of the average heat output (9.8 kW). Continuous ventilation in the emplacement drifts at the rate of 2 to 10 m^3/s would be required for the 50-year preclosure period.

One advantage of the SR reference design is that water mobilized by temperatures higher than boiling in rock near the emplacement drift would be diverted to drain through the cooler pillars between drifts, rather than collecting above the emplacement drift. The boiling fronts created by the water being driven away from the drifts by temperatures above 96°C are not expected to coalesce in this design. It is important to acknowledge, however, that for this design, it is unlikely that all condensate will drain away from the drift.

Recognizing that the SR reference is expected to evolve during the detailed design process, the initial configuration of the recommended design consists of the following major design features:

- Areal mass loading—60 MTU/acre
- Emplacement drift spacing—81 m (center to center)
- Entire emplacement in the upper block of the characterized repository—(about 1,060 acres)
- Total emplacement drift length—54 km
- Total access drift length—33 km

- Emplacement drift diameter—5.5 m
- Ground support—Steel
- Invert—Steel frame, with sand or gravel ballast
- Drift loading—Line loading, with 10 cm between waste packages
- Drip shields—Continuous 2 cm titanium Alloy Grade-7 (titanium-7); self-supporting
- Backfill—Granular material
- Waste package—2 cm thick Alloy-22 over 5 cm thick SS-316L, with a capacity of 21 PWR SNF assemblies
- Heat output—Average PWR waste package output of 9.8 kW, with blending to keep the hottest packages within 20 percent of the average
- Repository ventilation—Approximately 2 to 10 m^3/s continuous preclosure airflow in emplacement drifts for temperature control.

An areal mass loading of 60 MTU/acre, accomplished through closely spaced waste packages, line loading, and a drift spacing of 81 m, will fulfill both goals of the SR design.

Optimization of the Reference Design–This reference design will have to be optimized before it can be brought forward to the level of detail required for the SR and possible LA. The following design factors may be analyzed through sensitivity studies and the comparative results presented in the TSPA-SR.

Extended Ventilation and Time of Repository Closure–The reference design assumes the emplacement drifts will be actively ventilated for the 50-year preclosure period. However, the design should not preclude the possibility of operating the ventilation system for a longer period of time, if that should be necessary in the future. This option would allow maximum flexibility in case future changes to the postclosure thermal goals become necessary. Additional analyses will be performed to evaluate the impacts of longer preclosure ventilation periods on postclosure performance.

Waste Package Size–The CRWMS M&O design organizations will perform optimization studies on waste package sizes to determine if it is reasonable to provide an increased level of standardization for CSNF. Preliminary blending studies showed that fewer than 200 of the CSNF waste packages require the smaller, 12 PWR assembly capacity waste package. Derating (i.e., not completely filling the waste packages) could be considered for the 21 PWR/44 BWR assembly capacity waste package as a trade-off against developing two waste package sizes for CSNF. Optimization studies will have to consider the disposal of nonstandard CSNF fuel sizes such as South Texas fuel. If the optimization studies on waste package sizes indicate that increased standardization is warranted, additional analyses may be performed to evaluate the impacts on postclosure performance.

Single Corrosion Resistant Material Waste Package–The CRWMS M&O has recommended that the waste package design use Alloy-22 over stainless steel. However, models that include stainless steel as a barrier to waste package degradation may be developed and implemented.

Corrosion Resistant Material Canisters–The CRWMS M&O is considering an additional barrier for the small quantities of CSNF that do not have intact zirconium-based cladding. This additional barrier could also be considered for defense HLW that does not include a highly corrosion resistant barrier as part of its makeup (e.g., the vitrified glass logs). Analyses to evaluate the impacts of adding corrosion resistant material canisters to CSNF without intact zirconium-based cladding and to defense HLW that does not include a highly corrosion resistant barrier may be required.

Invert Design–The reference design includes a steel invert with granular ballast and steel ground support. Materials for the granular ballast have not been specified. Testing and analyses to determine the optimal material properties of the invert are underway. Analyses may be required to evaluate the postclosure implications of several invert materials.

Drip Shields–The drip shield design for the reference design is only preliminary and conceptual. Additional details will be needed to design a drip shield that can be defended in the licensing process and modeled adequately for TSPA. The materials and configuration for the drip shield will evolve, and the timing of the drip shield placement must be determined. Analyses may be required to evaluate the postclosure performance implications for different drip shield design and emplacement configurations.

Backfill–The reference design includes a granular backfill to protect the drip shields from rockfall and extend their life by controlling the relative humidity at their surfaces. Actual material properties or a specific backfill material have not been specified. Analyses may be required to evaluate the postclosure performance implications of several different backfill materials. Analyses of the postclosure implications of the reference design with backfill removed may be conducted as part of the TSPA-SR.

Additional Repository Capacity–The reference design is based on a 70,000 MTU capacity. In order to accommodate 70,000 MTU at 60 MTU/acre, approximately 1,060 acres of emplacement area are required. Recent requirements to the *Monitored Geologic Repository Requirements Document* (YMP 1999) include the ability to accommodate 86,700 metric tons of initial heavy metal of CSNF, 2,502 metric tons of initial heavy metal of DSNF (this includes 65 metric tons of initial heavy metal naval SNF), and 19,333 defense HLW canisters. The increased capacity would require approximately 1,450 acres of emplacement area. Analyses of the postclosure implications of the additional inventory and increased repository footprint will be required.

4.7 HUMAN INTRUSION ANALYSES

The TSPA-SR will present an evaluation of total system performance against the DOE's siting guidelines at 10 CFR 963. 10 CFR 963 is expected to invoke the environmental standards specified by the EPA 40 CFR 197 and the applicable implementing regulations set forth by the NRC proposed 10 CFR 63 (64 FR 8640). Until 10 CFR 963 is promulgated, TSPA-SR will be guided by available regulatory information from the proposed 10 CFR 63 (64 FR 8640).

Human intrusion generally is interpreted to mean inadvertent penetration of the repository (e.g., by drilling operations) that either releases radionuclides at the surface or accelerates radionuclide transport to the dose exposure location. The proposed NRC regulation, proposed 10 CFR 63 (64 FR 8640), specifies that the effect of an inadvertent human intrusion on the potential nuclear waste repository at Yucca Mountain should be evaluated separately from the nominal postclosure performance analyses. The proposed regulation also provides details about how the human intrusion is assumed to occur. The final version of proposed 10 CFR 63 (64 FR 8640) is expected to contain a requirement for the evaluation of a human intrusion scenario, similar to the requirement contained in the draft currently under review.

Human intrusion, as it will be modeled in TSPA-SR, is a special case in proposed 10 CFR 63 (64 FR 8640). The current wording in the supplemental information accompanying the proposed NRC regulation specifies a stylized scenario to "show that the repository exhibits some resilience to a breach of engineered and geologic barriers" (proposed 10 CFR 63 (64 FR 8640)). In modeling the stylized scenario, the performance measure will be the same as for the probabilistic TSPA, except that consideration of the probability of occurrence is not applied to consequences.

The proposed regulatory guidance for stylizing the human intrusion scenario (proposed 10 CFR 63 (64 FR 8640)) consists of:

- The human intrusion will occur at 100 years after repository closure.
- The intrusion will result in a nearly vertical borehole that breaches one waste package and extends down to the SZ.
- Assume current resource exploration practices for the diameter of the drill hole and the composition of the drilling fluid.
- Hazards to the drillers and the public from any material brought to the surface will not be evaluated. Instead, the dose to the average member of the critical group will be evaluated and should not exceed the regulatory limit.
- The open borehole will not be sealed adequately to prevent the infiltration of water.
- The NRC intends that the human intrusion analysis will show that the repository exhibits some resilience to a breach of the engineered and geologic barriers from events that are reasonably of concern.
- Results of the human intrusion calculation must be within the performance objective of 25 mrem/yr.

4.7.1 Total System Performance Assessment-Site Recommendation Human Intrusion Scenarios

For the TSPA-SR, this stylized conceptualization of inadvertent intrusion provides only a partial basis for the human intrusion scenario. To complete the scenario specification, additional assumptions are needed for the following parameters and processes:

- Size of the borehole
- Area and volume of waste exposed
- The nature of seepage into the borehole
- Inadequately sealed borehole permeability
- Amount of waste exposed to moisture
- Waste mobilization and transport processes.

For the purposes of capturing a range of consequences, two alternate conceptualizations of the release modes from human intrusion will be modeled (Table 4.7-1). Differences between the two conceptualizations, summarized in Table 4.7.1, involve different water contact mechanisms leading to waste mobilization.

Table 4.7-1. Possible Key Assumptions for Each Human Intrusion Case

Both Conceptualizations
Key Assumptions: Human Intrusion Occurs 100 Years After Repository Closure Effect of Human Intrusion Only, Dose From Rest of Repository Not Calculated Number of Radionuclides to be Tracked Needs to be Determined Type of Waste Package Breached Needs to be Determined
Release Mode 1
Description: Effect of Open and Unsealed Borehole and Advective Release
Key Assumptions: Increased Water Flow Through Waste Package as a Result of the Borehole Invert and UZ Barriers Compromised Cladding and Waste Form Degradation Same as TSPA-VA Base Case
Release Mode 2
Description: Effect of Breached Waste Package and Diffusive Release
Key Assumptions: Effect on Waste Package Corrosion Modeled, Minor Impact to Other Barriers Release is Due to Diffusion Through the Breach in the Waste Package Cladding and Waste form Degradation Same as TSPA-VA Base Case

In the first conceptualization, advective release is assumed to dominate the transport process through the waste package (Figure 4.7-1). The advective process waste mobilization model assumes that a hole the size of a standard rock bit (for water exploration and development) exists from the ground surface, through the drip shield and the waste package, and continues on to the water table. It is further assumed that waste is exposed within the package at the surface area created by an intrusion. Waste is assumed to slough off the exposed sides of the hole and collect in the bottom of the package, instead of falling to the bottom of the borehole. It is assumed that the water will contact the waste on the exposed sides of the hole through the package, as well as in the rubble at the bottom of the hole in the package.

There is the further assumption that water from base case rainfall rates enters the borehole, which serves as a fast path with an assumed percolation rate. All water that percolates down the borehole is assumed to enter the waste package and contact the waste. Mobilization of the waste is assumed to occur through advective processes. Water containing the waste is assumed to travel down the borehole, below the waste package at the same percolation rate as that for the borehole above the waste package. At the water table, the waste is transported by processes appropriate for SZ conditions.

In the second conceptualization, diffusive transport is assumed from the waste package (Figure 4.7-2). The diffusive process waste mobilization model assumes the same conditions for borehole penetration of the repository as the first model. However, in this scenario the borehole is modeled in the same manner as that for breach by corrosion caused patches in WAPDEG. A patch equivalent hole is assumed on the top and bottom of the waste package. The waste between the holes is assumed to be gone due to the human intrusion. Mobilization processes will assume diffusion from the waste package into the invert and the continuation of the borehole, which is assumed to be filled with rubble similar to the natural conditions of the UZ. At the water table, the waste is transported by processes appropriate for SZ conditions.

These two alternate conceptualizations of radionuclide release will provide a range of possible consequences of human intrusion. Attributes of the system, such as thermal effects that could drive water away from the drifts and thus prevent seepage through the unsealed borehole, the overall seepage rate (consistent with the base case), and the lack of impact on adjacent waste packages arising from the damage to one package will be evaluated. Model parameters can be chosen to be specific to Yucca Mountain. Parameters used for the human intrusion scenario will be within ranges used in the probabilistic TSPA-SR analysis.

4.7.2 Modeling Issues

Given the requirements provided in the proposed regulation (proposed 10 CFR 63 (64 FR 8640)), several modeling issues have been identified that may have an effect on total system performance. The following paragraphs describe these issues.

The first issue concerns the number of radionuclides that need to be tracked to the accessible environment for the human intrusion scenario. For the TSPA-VA base case (CRWMS M&O 1998a, Chapter 6), nine radionuclides were selected for transport modeling and dose calculations based on their half-lives and transport properties through the natural barrier systems. The first package failure for the TSPA-VA base case was assumed to occur at 1,000 years (CRWMS M&O 1998a, Chapter 11), by which time many of the short-lived radionuclides will have decayed to insignificant levels. Other radionuclides with intermediate half-lives are strongly sorbed in the UZ, the SZ, or both, and, therefore, are unlikely to travel in significant concentrations out to the accessible environment. The human intrusion scenario for TSPA-SR is required to occur at 100 years. Because the engineered and natural barriers will be compromised, and because of the early timing of the human intrusion event, it is expected that several additional radionuclides will need to be considered to properly estimate the dose rates at the location of the critical group (i.e., 20 km). Radionuclides that are important in the human intrusion scenario will be identified so that they may be incorporated into the total system model.

The SZ transport model uses a convolution method employing breakthrough curves to calculate radionuclide concentrations at the accessible environment at the end of the SZ. If new radionuclides are identified as being potentially important, new radionuclide specific breakthrough curves will need to be generated. Also, the current convolution method does not allow for ingrowth in decay chains. If the use of decay chains is determined to be necessary, the SZ transport model will require modification.

The possible effect of the borehole on UZ flow above and below the repository may need to be evaluated. A first step in determining the impact of the borehole would be to identify the assumed properties of the borehole. Flow through an open borehole would be different than flow through a borehole that is rapidly filled with debris. Once the properties of the borehole are determined, flow modeling may need to be conducted to determine the actual impact of the borehole above and below the repository level on SZ flow.

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5.2 CODES, STANDARDS, AND REGULATIONS

10 CFR (Code of Federal Regulations) 60. Energy: Disposal of High-Level Radioactive Wastes in Geologic Repositories. TIC: 232902.

10 CFR 960. Energy: General Guidelines for the Recommendation of Sites for Nuclear Waste Repositories. TIC: 238500.

40 CFR 191. Protection of Environment: Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes. TIC: 238620.

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5.3 PROCEDURES

AP-2.13Q, Rev. 0, ICN 0. *Technical Product Development Planning*. ACC: MOL.19990701.0617.

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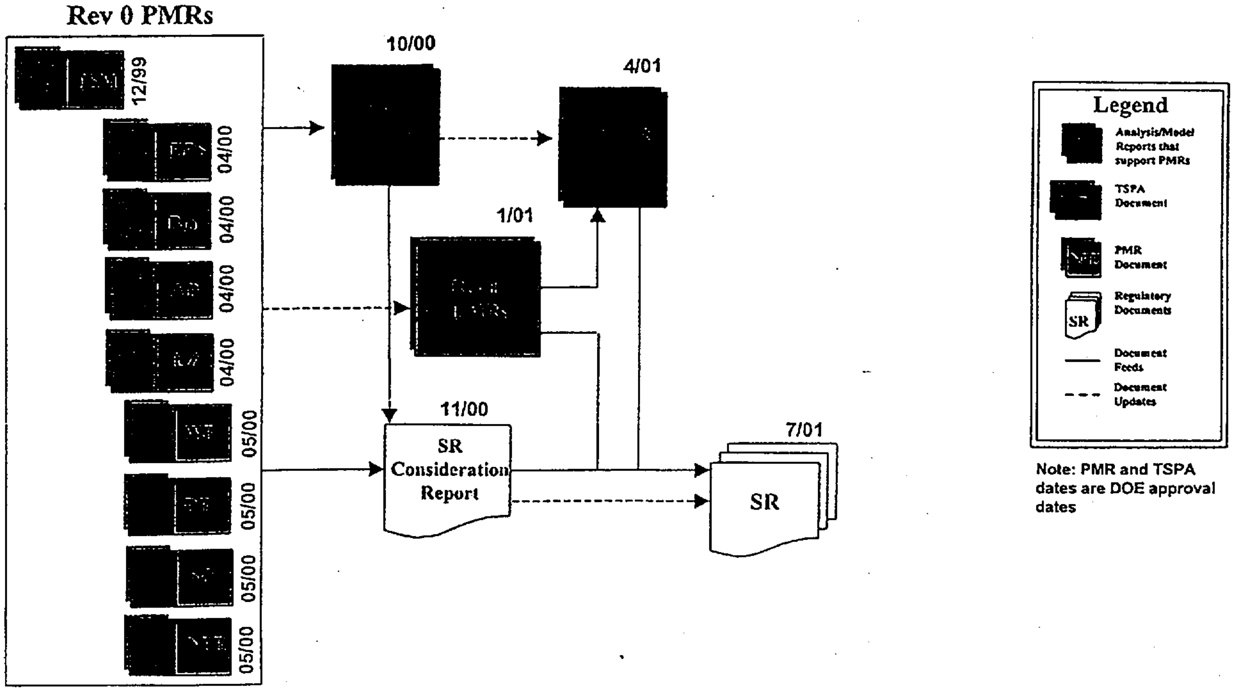

Note: PMR and TSPA dates are DOE approval dates

Figure 1.5-1. Linkage of Major Programmatic SR Milestones

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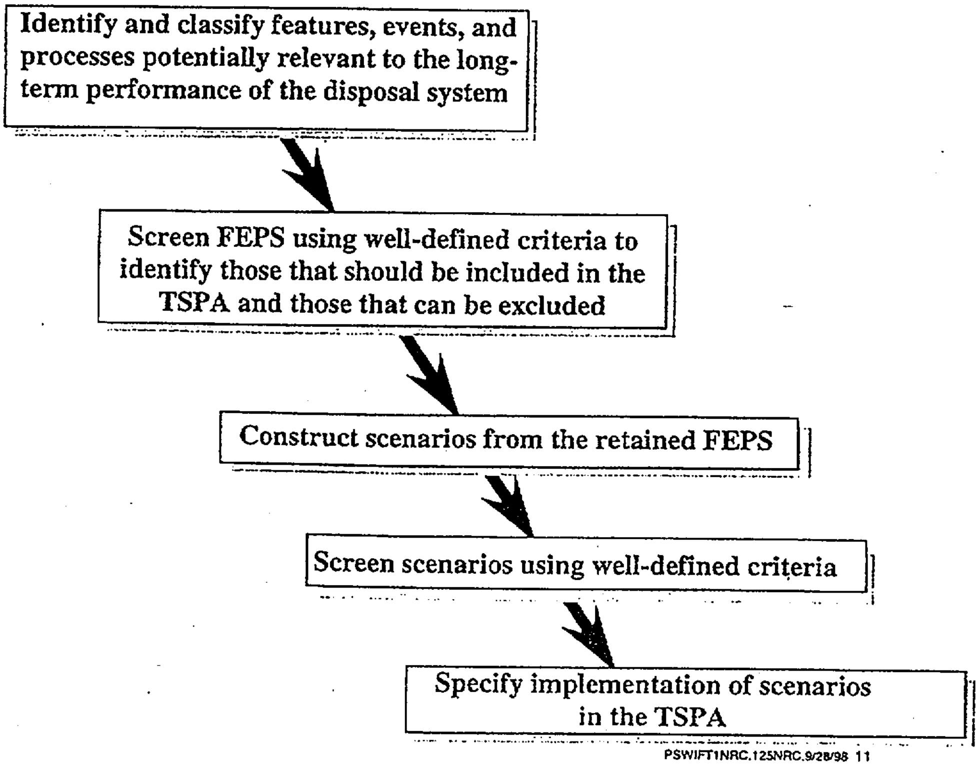

Figure 2.2-1. The Five Steps in Scenario Development

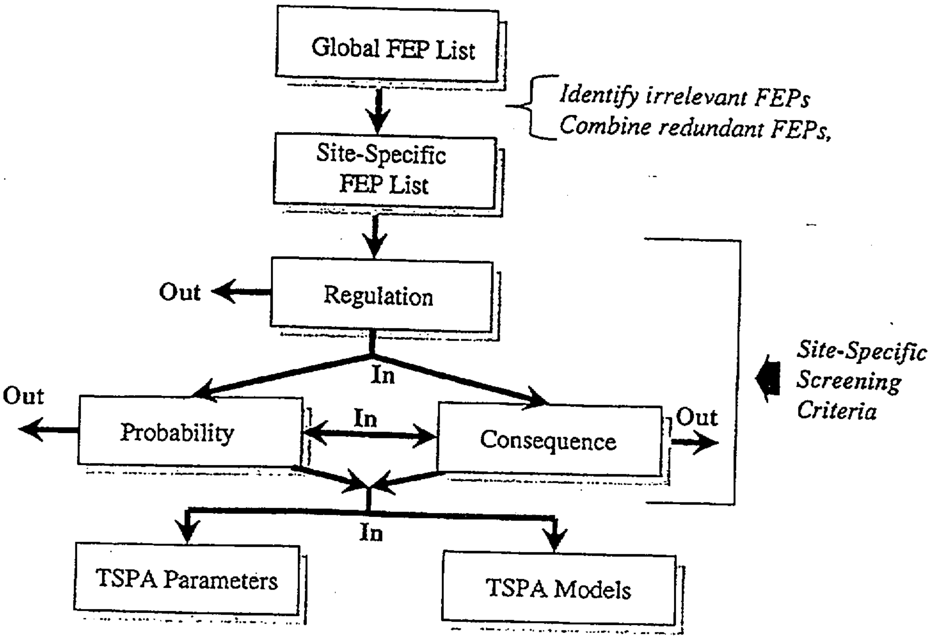

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Figure 2.2-2. Schematic Illustration of the FEP Screening Process

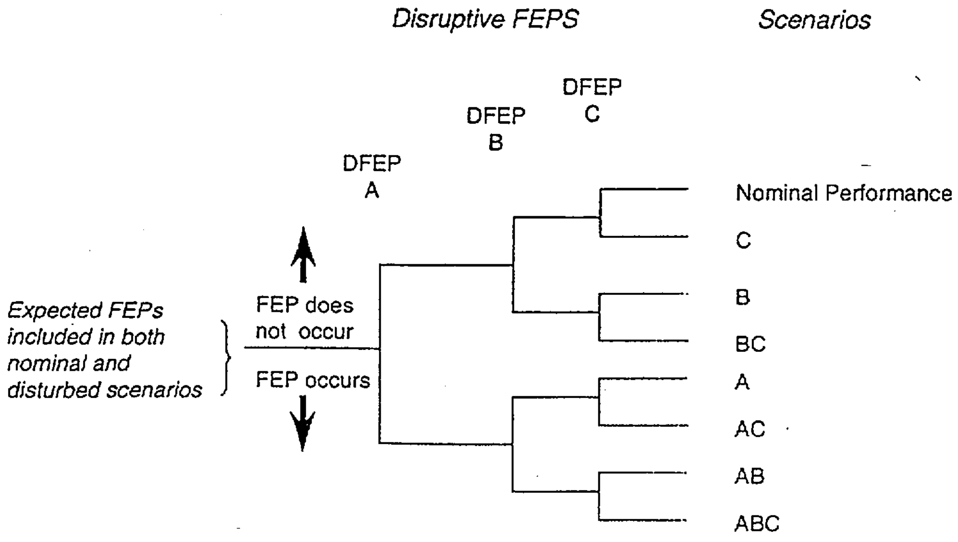

Figure 2.2-3. Example Logic Diagram Showing Scenarios Formed by all Combinations of the Occurrence and Nonoccurrence of Three Disruptive Events (DFEPs A, B, and C)

	A		(A)	
	B	(B)	B	(B)
C	ABC	AC	BC	C
(C)	AB	A	B	Nominal Performance

Legend:

A = DFEP A occurs
(A) = DFEP A does not occur

NOTE: The scenarios displayed here are identical to those displayed in Figure 2.2-3.

Figure 2.2-4. Example Latin Square Diagram Showing Scenarios Formed by all Combinations of the Occurrence and Nonoccurrence of Three Disruptive Events (DFEPs A, B, and C)

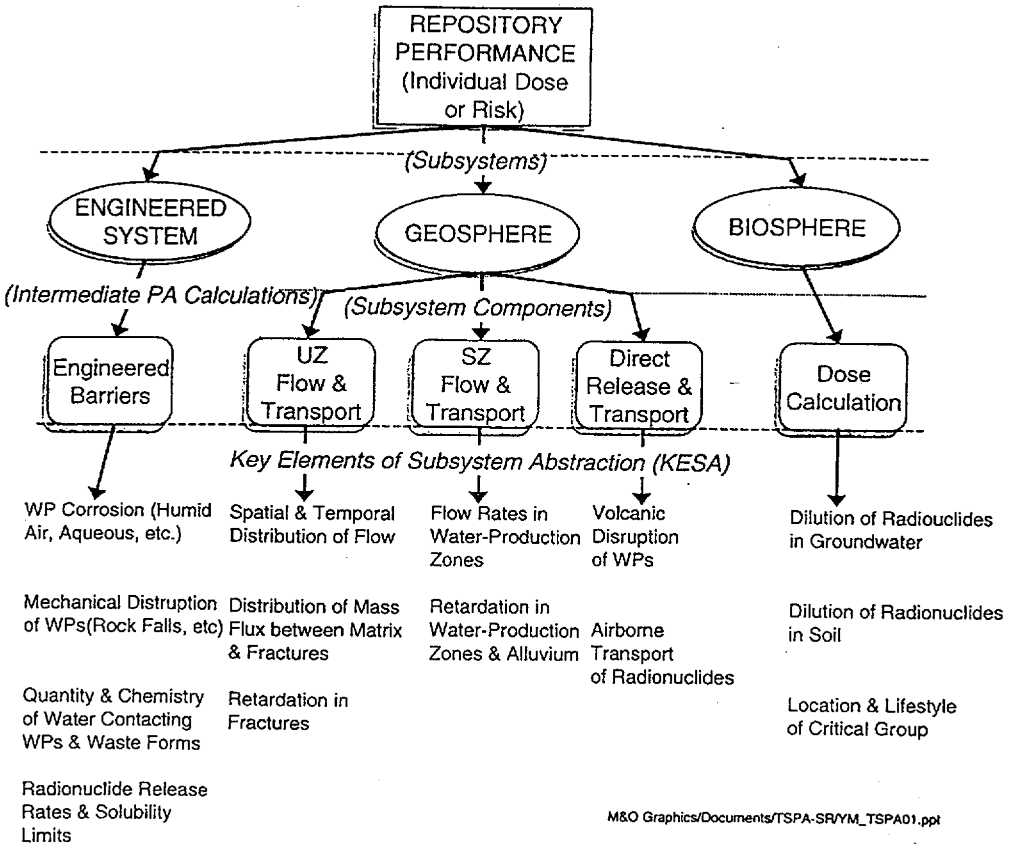

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Figure 2.3-1. Repository Performance

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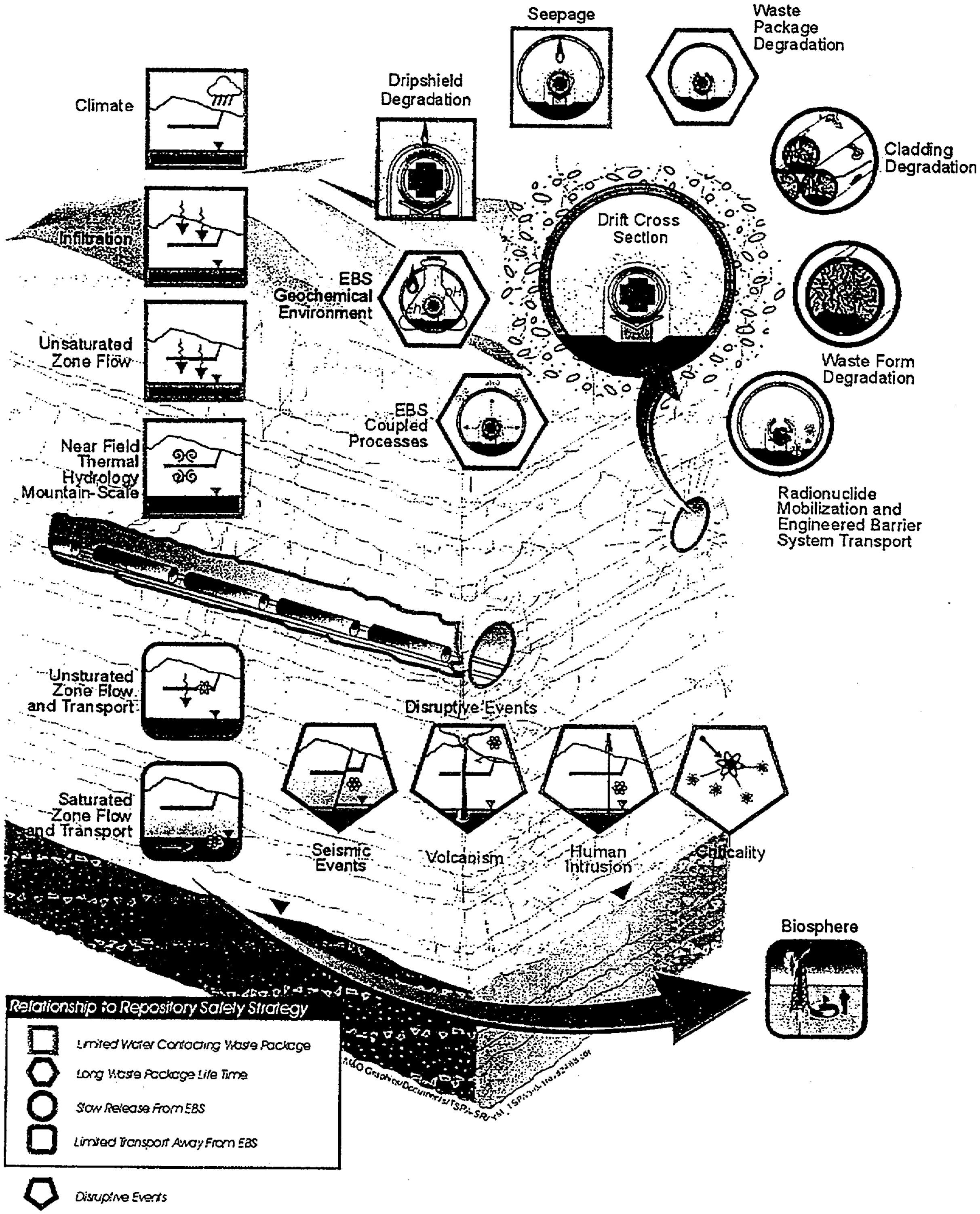


NOTE: Shown are the individual component models and submodels that together must be analyzed in evaluating the behavior of the Yucca Mountain repository system. These components comprise the individual building blocks of the TSPA analysis. The components are correlated to the four attributes of the repository safety strategy.

Figure 3-1. Major Components of the Total System Performance Assessment Model

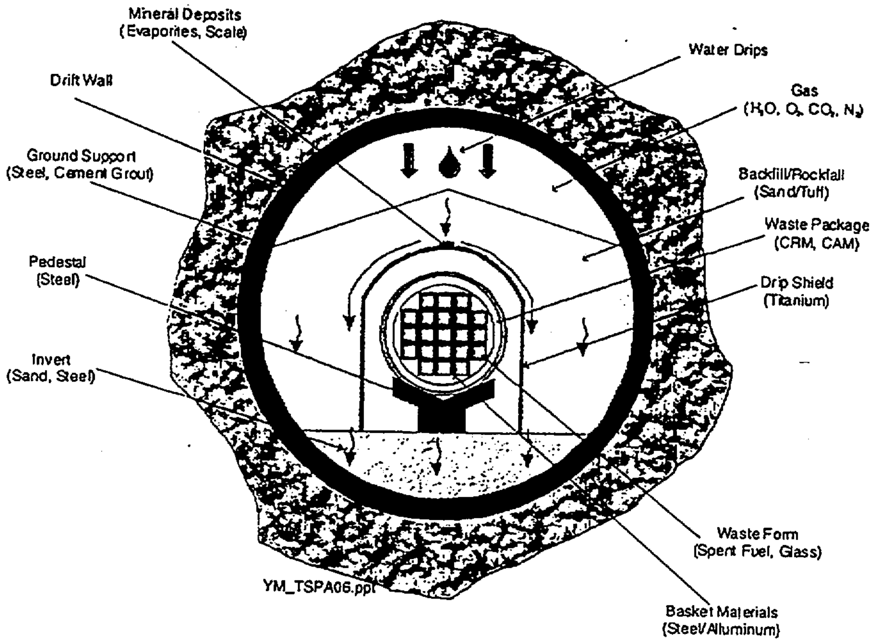


Figure 3.3-1. Schematic of Drift Conditions

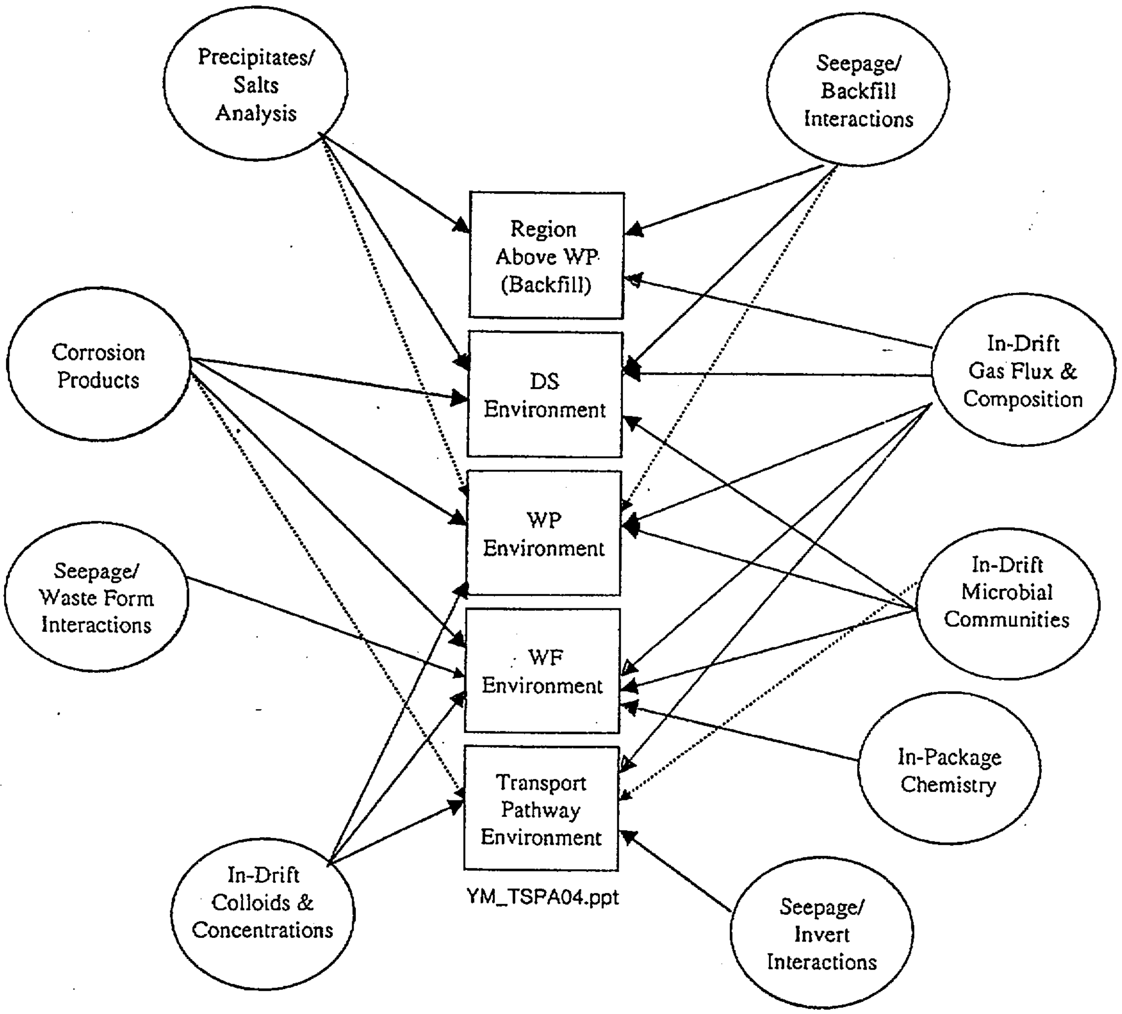


Figure 3.3-2. In-Drift Geochemical Modeling

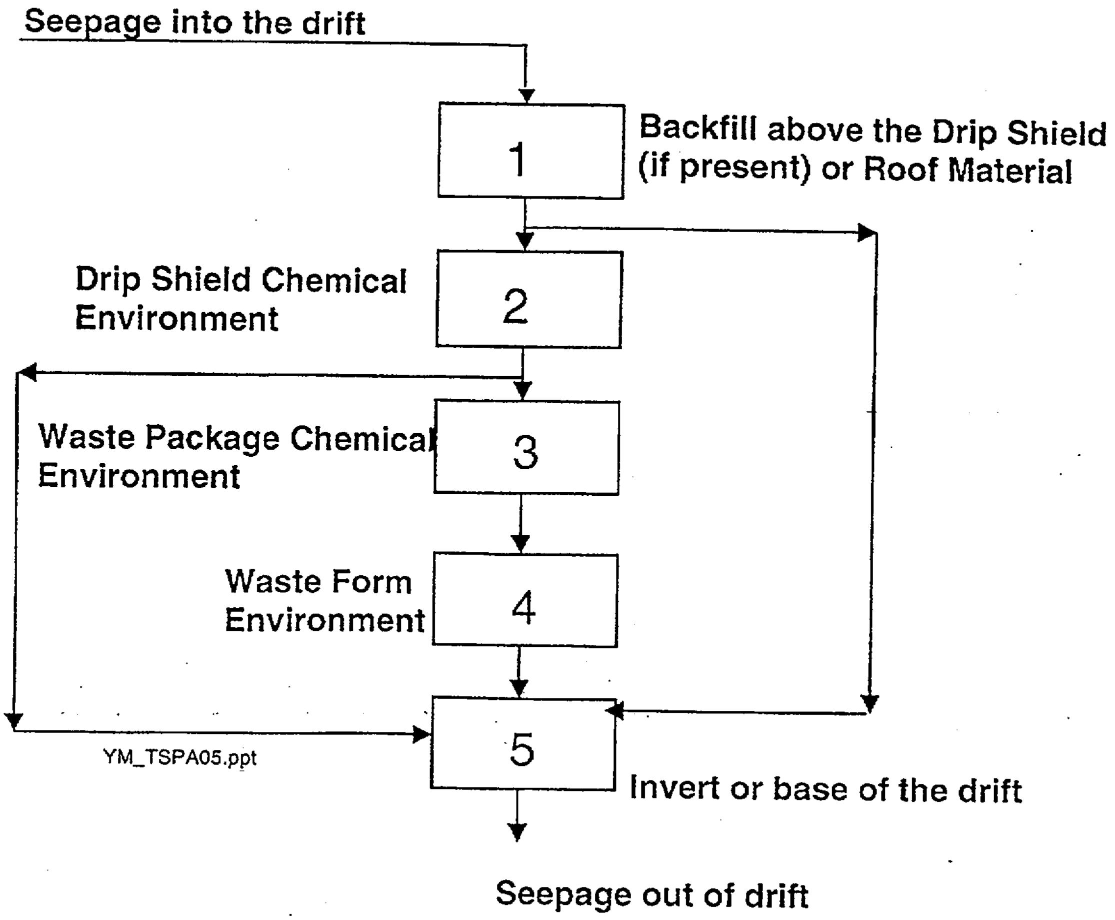
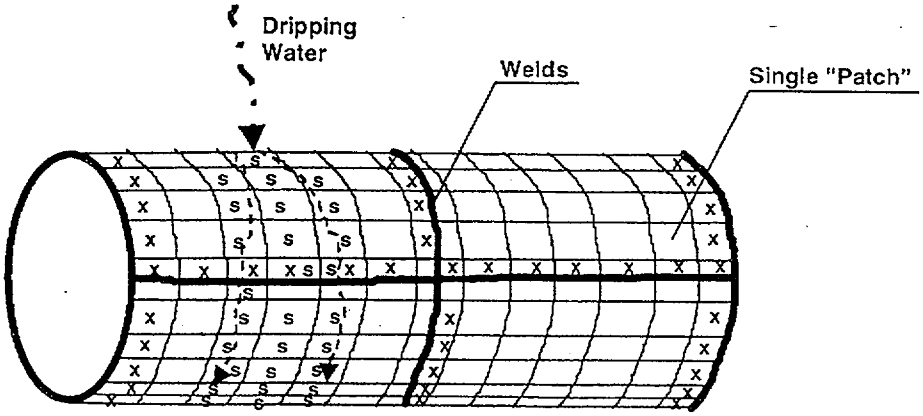


Figure 3.3-3. Identification of Key Locations for In-Drift Geochemical Model

* T, RH, in-drift water dripping
across repository from
drift-scale T-H model abstraction

* pH, [Cl] of dripping water & $P(O_2)$
across repository from
in-drift geochemistry abstraction



s - Patches with drips;
Potential salt deposits;
CRM localized corrosion

x - Patches with welds

Figure 3.4-1. A Schematic Illustrating the Conceptual Model for the Waste Package Degradation Modeling with the "Patches" Approach

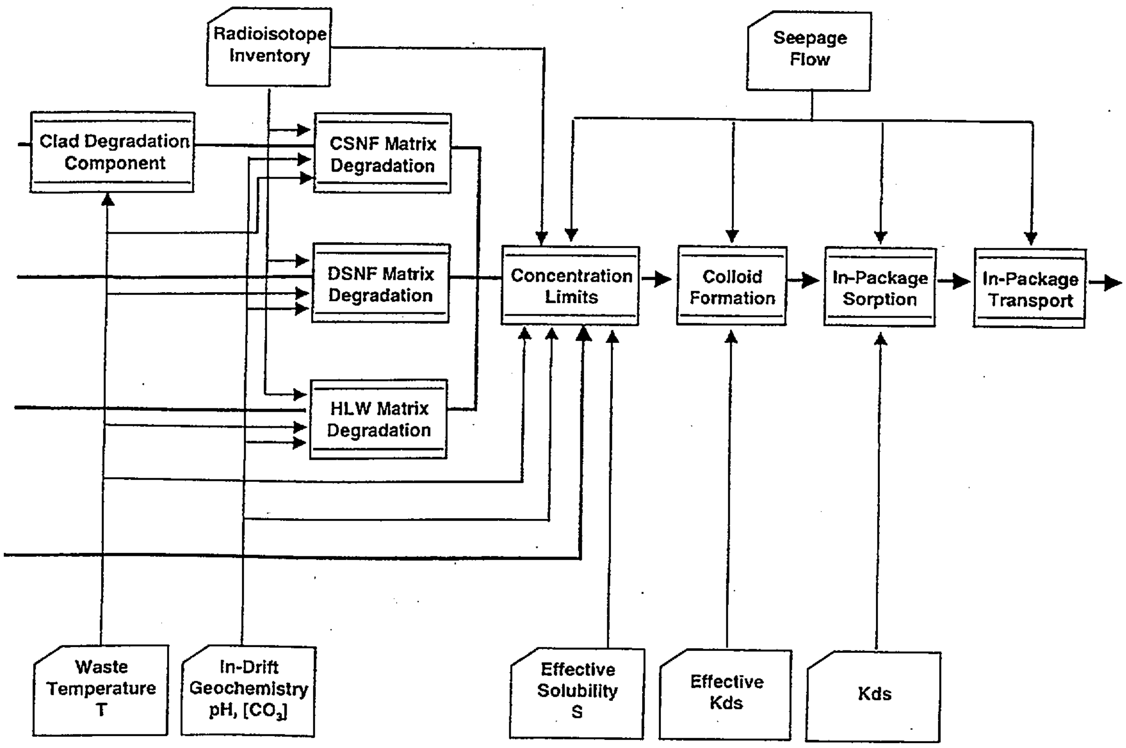


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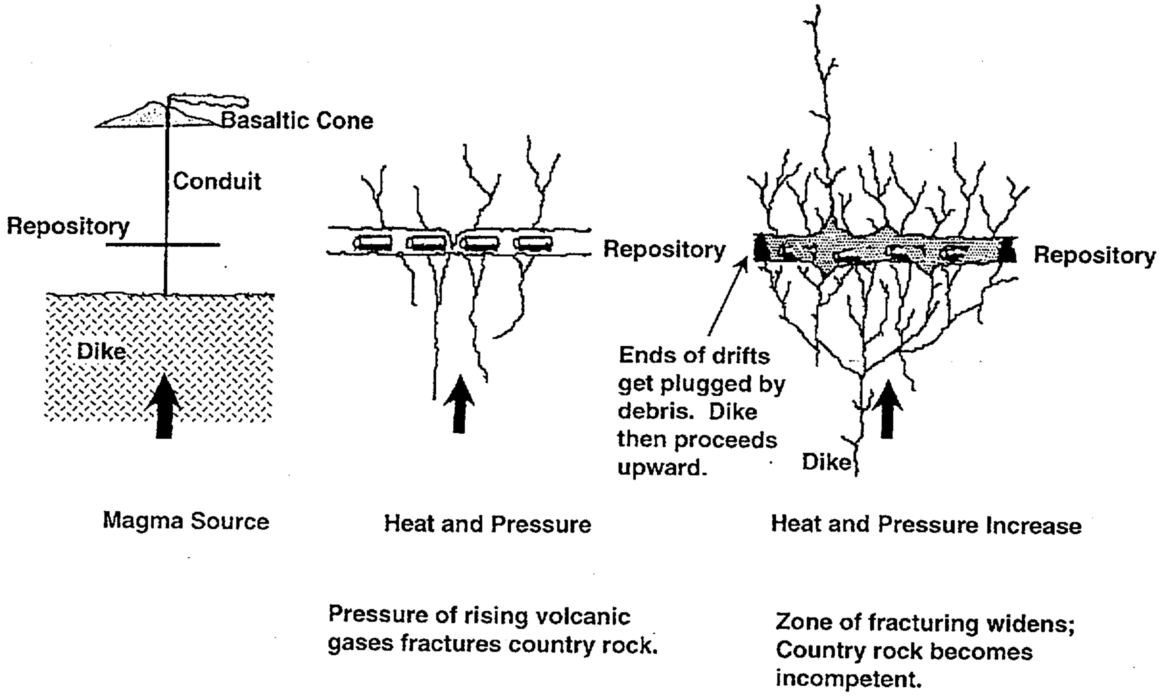
Figure 3.5-1. Major Components and Input of Waste Degradation Model



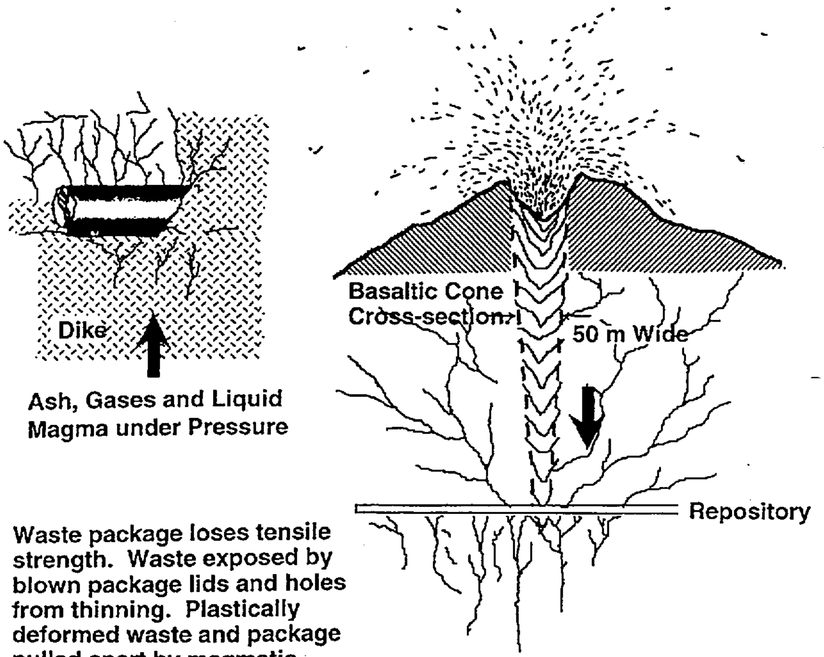
Ends of drifts get plugged by debris. Dike then proceeds upward.

Pressure of rising volcanic gases fractures country rock.

Zone of fracturing widens; Country rock becomes incompetent.

YM_TSPA16.ppt

Figure 3.9-1a. Conceptual Model for Magmatic Interaction with Repository



Eventually the conduit widens from the ground surface downward to as much as much as 50 m. The waste packages and the waste within the conduit diameter could be entrained an eruption stream. Waste form particles at the surface are assumed to be a wide range of diameters.

Waste package loses tensile strength. Waste exposed by blown package lids and holes from thinning. Plastically deformed waste and package pulled apart by magmatic flow processes. Waste becomes entrained in magma.

Conduit develops as an opening from surface downward as fractured rock is ejected.

YM_TSPA17.ppt

Figure 3.9-1b. Conceptual Model for Magmatic Activity (Continued)

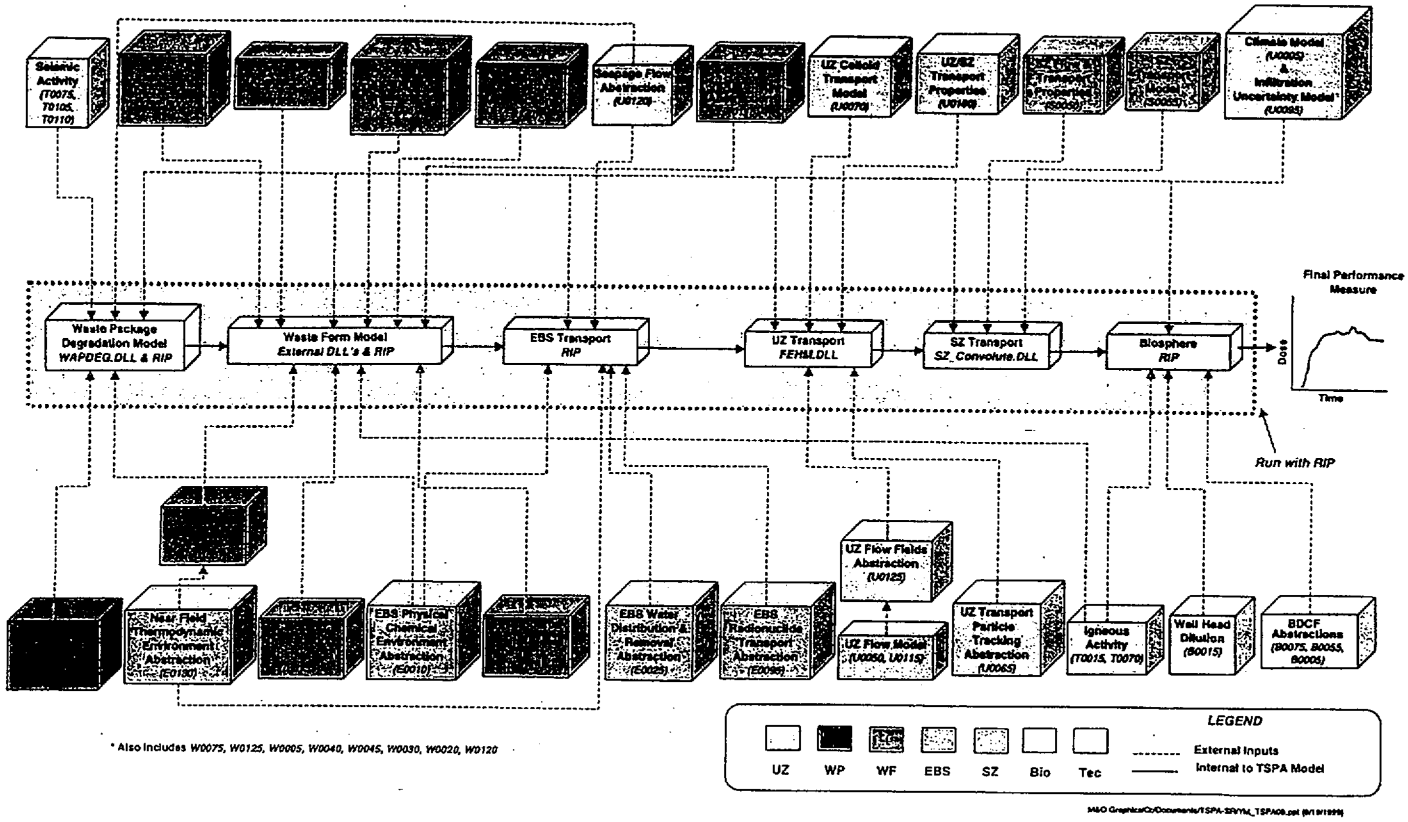


Figure 3.10-1. Total System Performance Assessment Model

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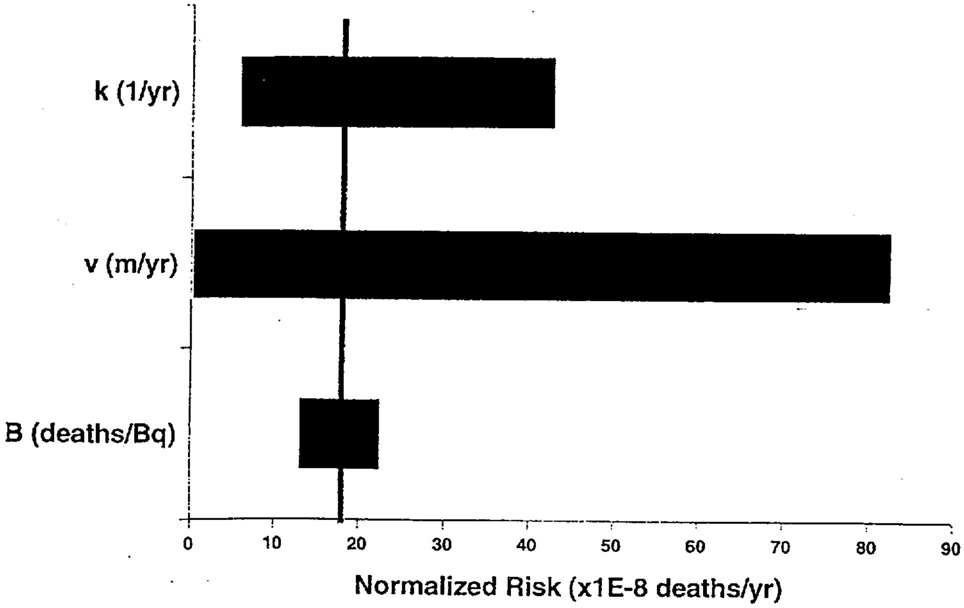
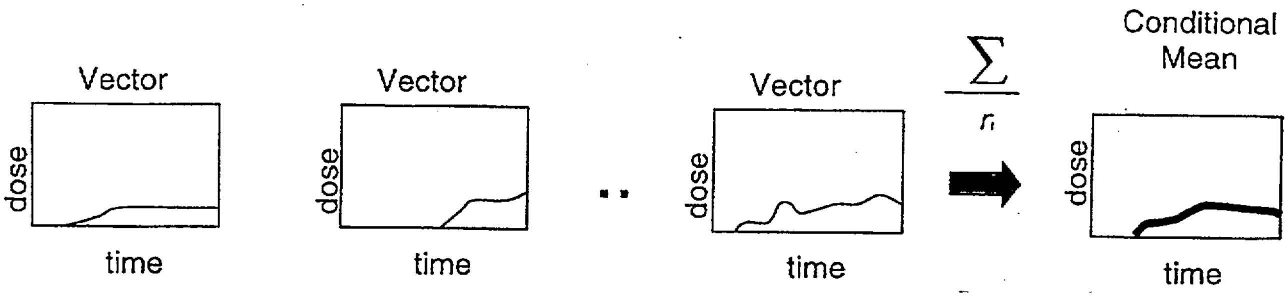


Figure 4.1-1. Example Tornado Chart, Showing Sensitivity of Predictions of a Health Risk Model to ±2σ Change in Its Parameters, as Compared to the Nominal Value (Boldline)



YM_TSPA13.doc

Figure 4.4-1. Constructing a Conditional Mean Dose History for a Single Scenario

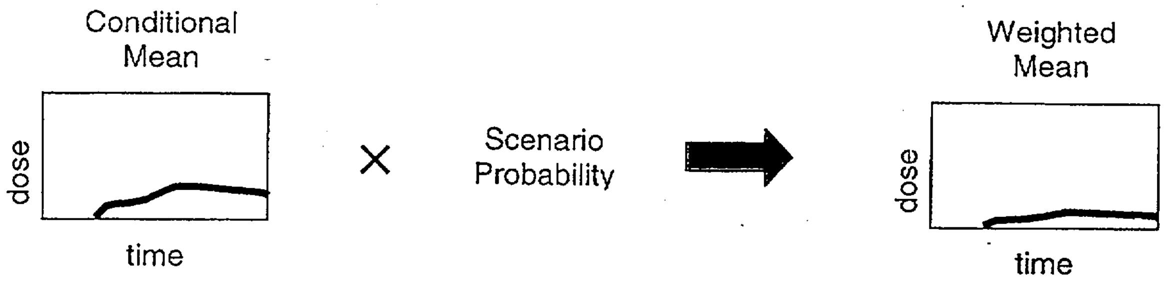


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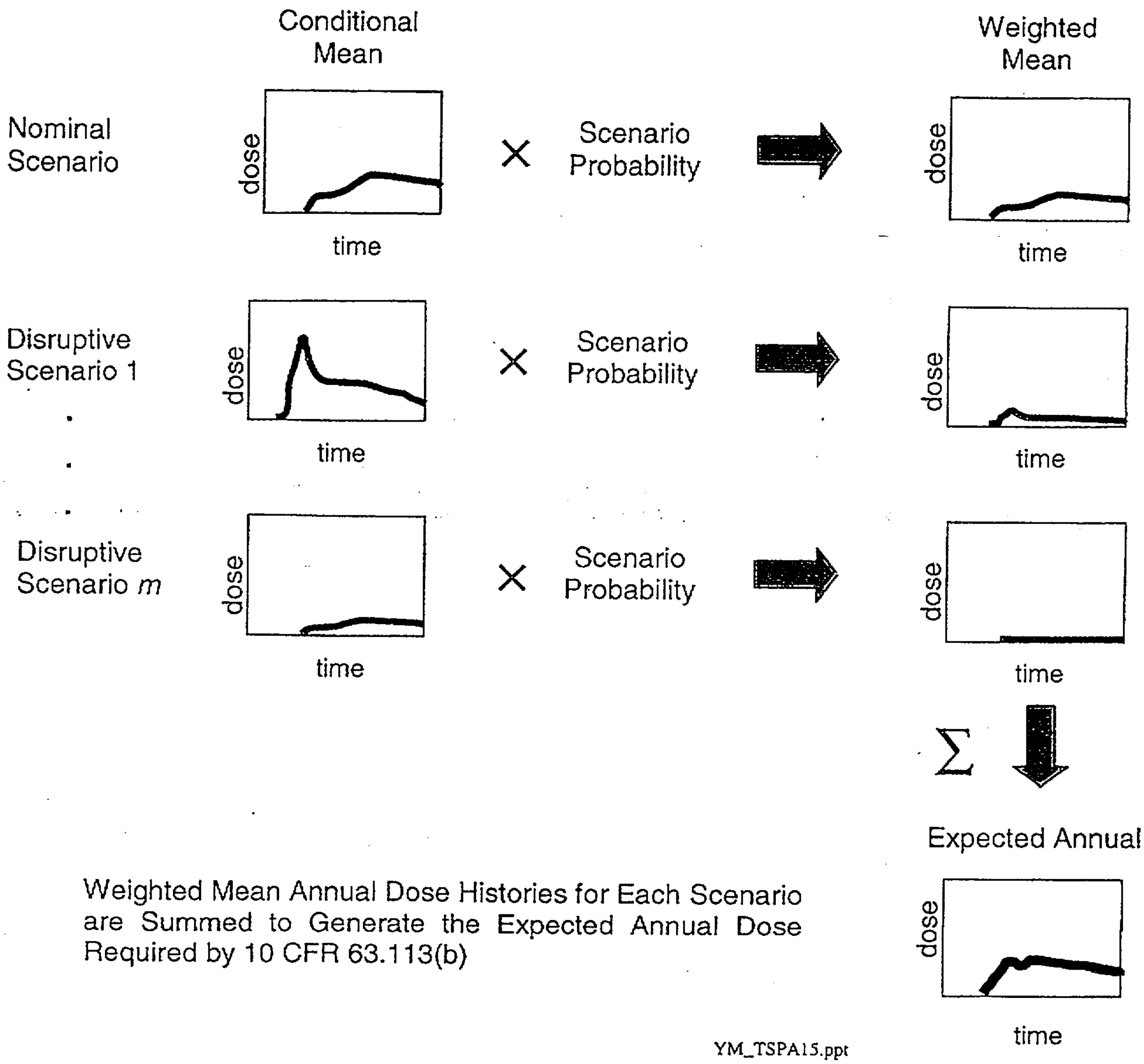
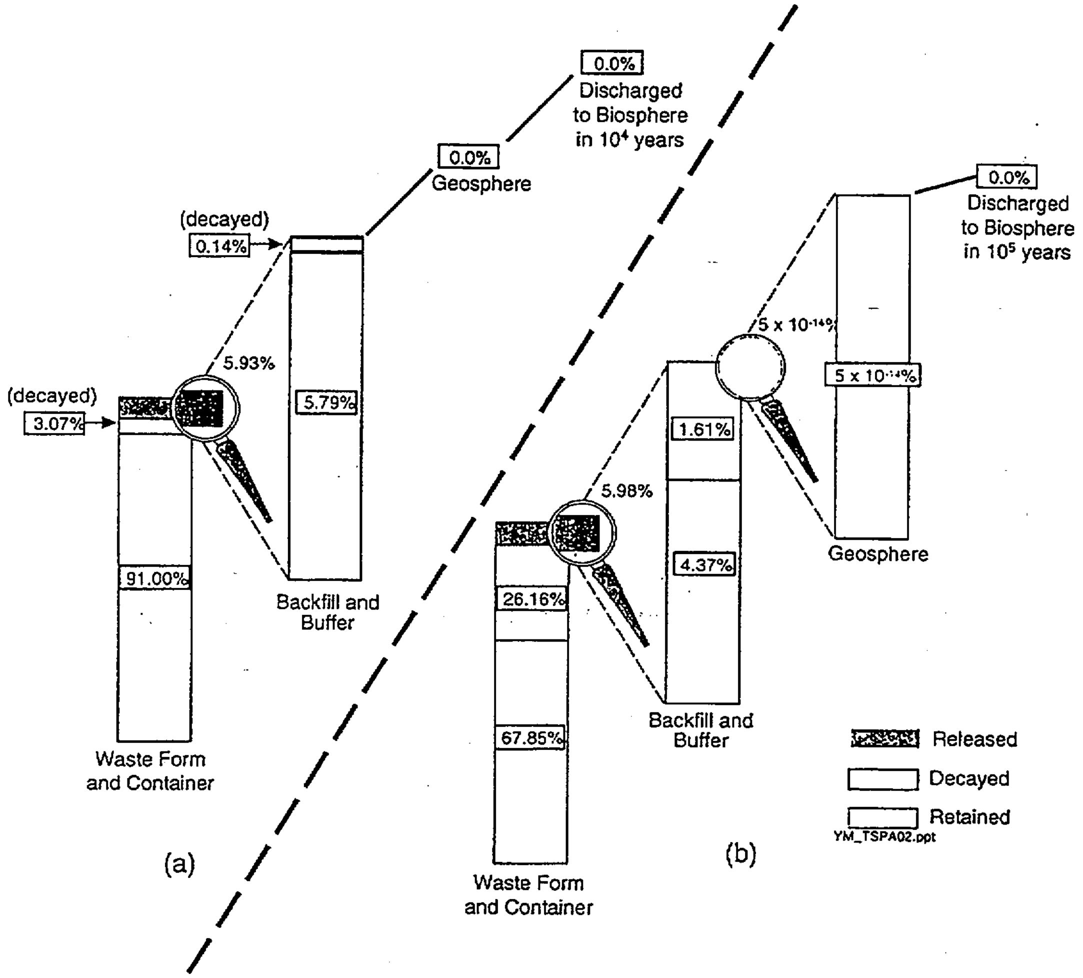
Figure 4.4-2. Multiplying the Conditional Mean Dose History by the Scenario Probability to Calculate the Probability Weighted Dose History for Each Scenario



Weighted Mean Annual Dose Histories for Each Scenario are Summed to Generate the Expected Annual Dose Required by 10 CFR 63.113(b)

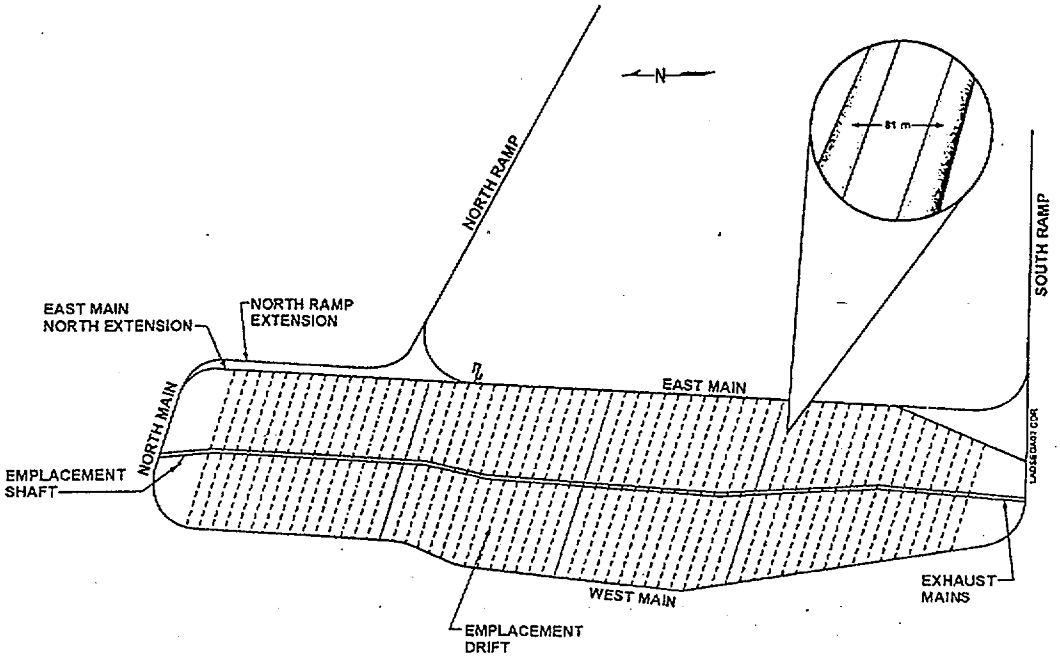
YM_TSPA15.ppt

Figure 4.4-3. Summing the Probability Weighted Annual Dose Histories for Each Scenario to Generate the Expected Annual Dose Required by Proposed 10 CFR 63.113(b) (64 FR 8640)



NOTE: Example shown is taken from Goodwin et al. (1994) and depicts the distribution of Tc99 in the disposal system after (a) 10,000 years and (b) 100,000 years.

Figure 4.5-1. Graphical Depiction of Barrier Effectiveness Computed with the BEF1 Metric



EDA 2: 60 MTU/ACRE - 81 M Center to Center

Figure 4.6-1. Plan View of Repository

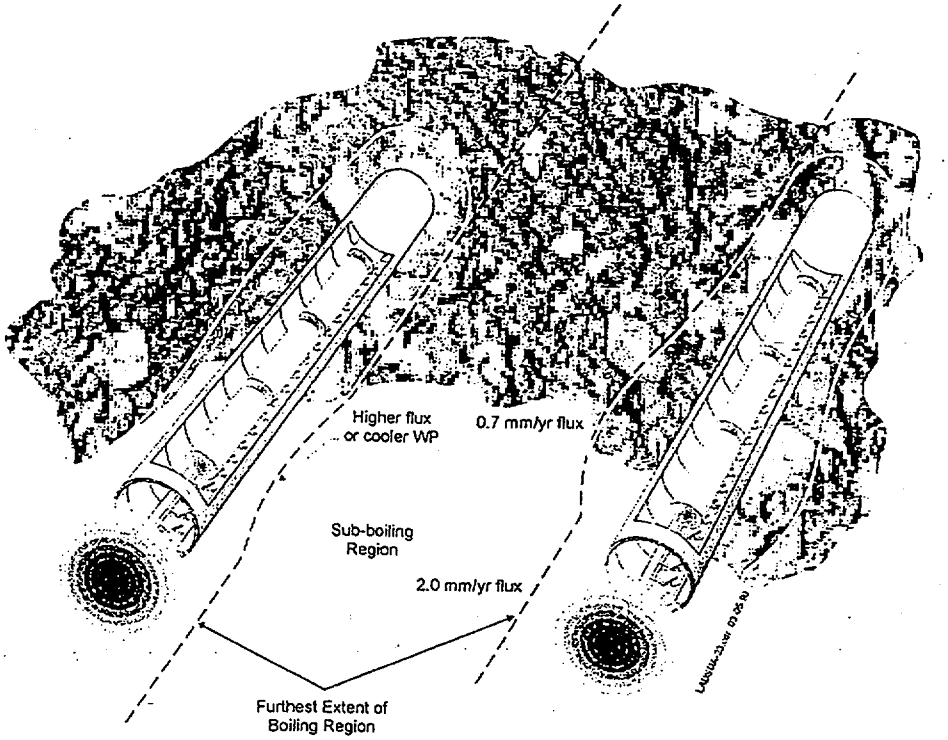
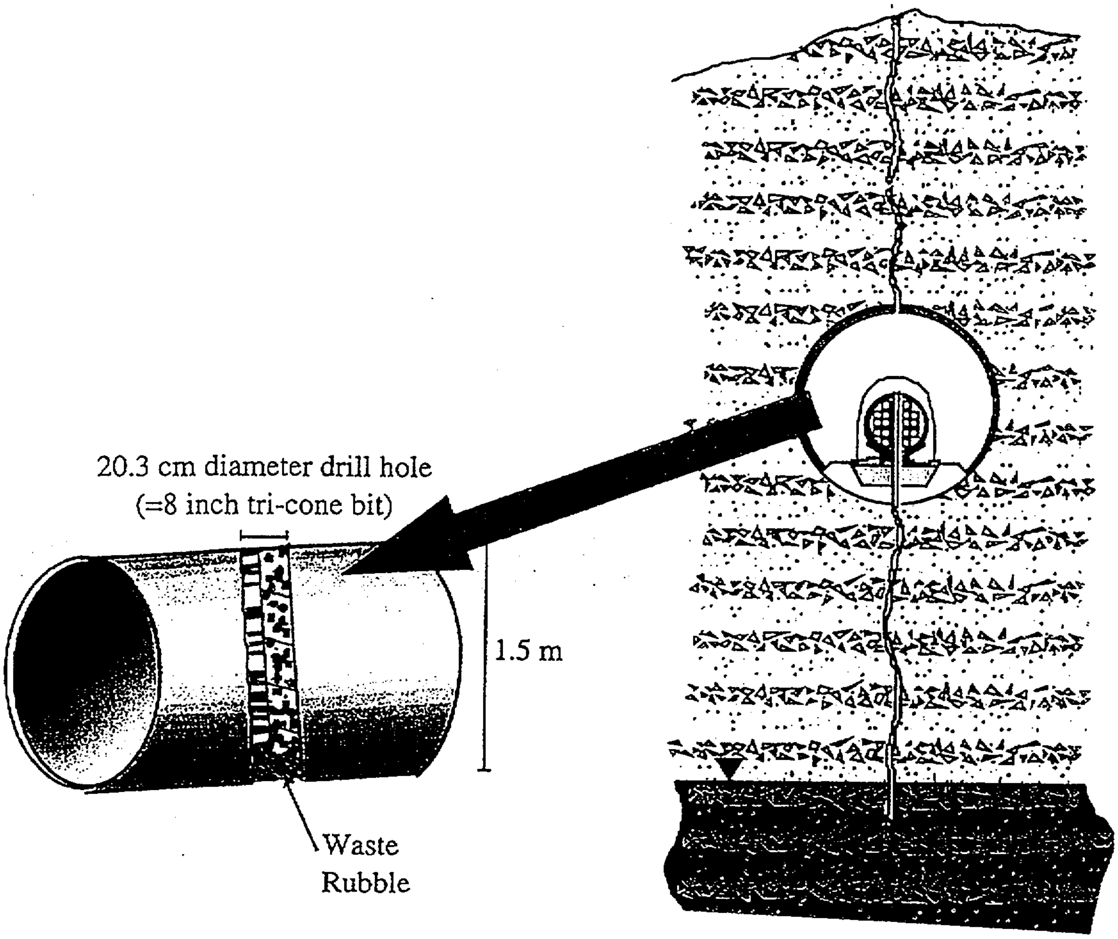


Figure 4.6-2. Schematic of Drift Showing Boiling Regions



Cutaway representation of a drill hole through a basket of fuel rods.

YM_TSPA09.ppt

Figure 4.7-1. Human Intrusion Scenario Advective Flow Into Package

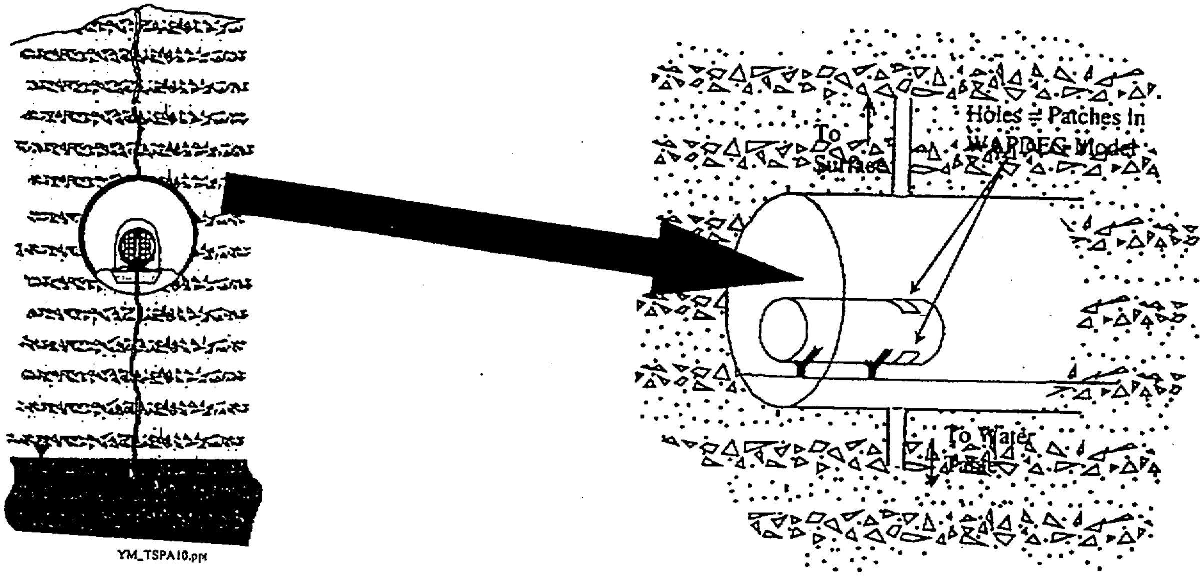


Figure 4.7-2. Human Intrusion Scenario–Diffusive Processes Mobilized Waste

APPENDIX A

GLOSSARY

APPENDIX A

GLOSSARY

Disruptive FEP (DFEP)–A retained FEP that has a probability of occurrence during the period of performance less than 1.0 (but greater than the cutoff of $10^{-4}/10^4$ year defined by the NRC at proposed 10 CFR 63.114(d) (64 FR 8640)).

Disruptive scenario–Any scenario that contains all expected FEPs and one or more disruptive FEPs.

Event–A natural or anthropogenic phenomenon that has a potential to affect disposal system performance and that occurs during an interval that is short compared to the period of performance.

Expected FEP (EFEP)–A retained FEP that, for the purposes of the TSPA, is assumed to occur with a probability equal to 1.0 during the period of performance.

Feature–An object, structure, or condition that has a potential to affect disposal system performance.

FEP–A feature, event, or process.

Future–A single, deterministic representation of the future state of the system. An essentially infinite set of futures can be imagined for any system.

Nominal scenario–The scenario that contains all EFEPs and no DFEPs.

Process–A natural or anthropogenic phenomenon that has a potential to affect disposal system performance and that operates during all or a significant part of the period of performance.

Retained FEP–An FEP that is identified by the screening process as requiring analysis in the quantitative TSPA.

Scenario–A subset of the set of all possible futures of the disposal system that contains futures resulting from a specific combination of FEPs.

Scenario class–A set of scenarios that share sufficient similarities that they can usefully be aggregated for the purposes of a specific analysis.

Seepage–the inflow of groundwater moving in fractures or pore spaces of permeable rock to an open space in the rock such as a drift. Specifically, the amount of percolation flux that enters the drift in a given time period. An important factor in waste package degradation and mobilization and migration of radionuclides out of the repository.

Seepage fraction–is the fraction of waste packages or drip shields contacted by dripping water.

Seep flow rate–is the average flow rate of water onto those waste packages or drip shields that have dripping.

Subscenario–A subset of a scenario (or a scenario class) created by defining one or more of the component FEPs more narrowly.