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TOTAL SYSTEM PERFORMANCE ASSESSMENT 1995 AUDIT REVIEW

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1 INTRODUCTION

1.1 BACKGROUND

The Department of Energy (DOE) recently issued the third in a series of reports on total system performance assessments (TSPAs) for the proposed high-level waste (HLW) repository at the Yucca Mountain (YM) site. This third iteration is documented in the report entitled "Total System Performance Assessment—1995: An Evaluation of the Potential Yucca Mountain Repository" (TRW Environmental Safety Systems, Inc., 1995). The report, referred to herein as TSPA-1995, presents the DOE performance assessment (PA) approach, assumptions, data, and the principal findings of the evaluation. Overall system performance is quantified in the DOE report in terms of both cumulative release and peak dose.

The technical evaluation contained in TSPA-1995 is distinct from the previous DOE iteration, designated TSPA-1993 (Wilson, et al., 1994), in a number of respects. Perhaps the three most significant differences are that the current iteration: (i) incorporates additional site data [e.g., U.S. Geologic Survey (USGS) infiltration map]; (ii) considers a variety of design options (e.g., thermal load, backfill, alternative corrosion model); and (iii) does not consider disruptive events such as seismicity, volcanism, and human intrusion. The current TSPA iteration also includes the extensive use of detailed process and abstracted models. New abstracted models have been developed for analyzing:

- Drift scale thermal-hydrologic behavior
- Waste package (WP) degradation
- Near-field unsaturated zone aqueous flux
- Unsaturated-zone flow and transport

In accordance with the Nuclear Regulatory Commission (NRC) Overall Review Strategy (Johnson, 1993), NRC has conducted an audit (or screening) review of the DOE TSPA-1995 report. This audit review contains major technical comments of the NRC and the Center for Nuclear Waste Regulatory Analyses (CNWRA) on TSPA-1995. These comments form the basis for identifying the TSPA methodology issues and were discussed at the NRC/DOE Technical Exchange Meeting, May 22–23, 1996. In addition, this review should form the basis for resolution of TSPA methodology issues.

1.2 OBJECTIVES OF THE AUDIT REVIEW

In contrast to previous audit reviews of DOE TSPAs, NRC has selected very specific topical areas for technical review which were considered to be of key importance to the calculation of total system performance. The primary objectives of this audit review are three-fold:

- Identify significant differences among the NRC approaches to total system PA and those presented in TSPA-1995
- Identify areas for future detailed review and independent analysis by NRC/CNWRA
- Contribute to the formulation of strategies for resolution of differences in TSPA approaches

Achieving these objectives will allow NRC and CNWRA staffs to focus on resolution of technical issues in relation to their importance to overall system performance. In addition, fulfilling these objectives will provide the basis for early feedback to DOE regarding NRC staff requirements for additional supporting information and clarifications necessary to accomplish detailed reviews of DOE TSPAs.

1.3 NUCLEAR REGULATORY COMMISSION KEY TECHNICAL ISSUES

To more effectively conduct its prelicensing activities, NRC has refocused its regulatory program on ten Key Technical Issues (KTIs). These KTIs, which are summarized in Table 1-1, were identified through a combination of: (i) iterative performance assessment (IPA), (ii) a systematic regulatory analysis of the Code of Federal Regulations (CFR) Title 10, Part 60 (10 CFR Part 60), (iii) a review of the DOE draft Waste Containment and Isolation Strategy (TRW Environmental Safety Systems, Inc., 1995), and (iv) NRC staff understandings of geologic processes and events relevant to the YM site. Each of these KTIs encompasses a number of subissues that NRC uses to guide its program and resolution of the principal issues. At present, NRC and DOE have agreed on the potential significance of eight of the ten KTIs. The two KTIs where DOE differs with NRC are igneous activity (i.e., volcanism) and structural deformation and seismicity.

Technical activities being conducted within these ten KTIs are providing the bases for development of acceptance criteria for compliance determination, and for interactions with DOE and other parties, with the central objective of issue resolution (Federline et al., 1996).

Table 1-1. Ten Key Technical Issues

Title
Total System Performance Assessment and Technical Integration
Igneous Activity (Volcanism)
Unsaturated and Saturated Flow Under Isothermal Conditions
Thermal Effects on Flow
Container Life and Source Term
Structural Deformation and Seismicity
Evolution of the Near-Field Environment
Radionuclide Transport
Repository Design and Thermal-Mechanical Effects
Support Development of the EPA Standard and NRC Regulation

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1.4 REVIEW APPROACH

In this audit review, a two-level review process was used that involved: (i) probing individual performance analyses relevant to the DOE Waste Containment and Isolation Strategy (WCIS) and (ii) conducting a broad review of TSPA-1995 methodology and calculational results to compile general comments regarding the DOE performance evaluation. In the first level, five primary review topics were evaluated by NRC and CNWRA staffs, namely:

- Subsystem Abstractions
- Infiltration and Deep Percolation
- Groundwater Dilution
- Calculation of Temperature and Relative Humidity
- Waste Package Failure Modes

These review topics were selected because of their importance to the WCIS and because the NRC and CNWRA staffs have performed significant technical studies on these topics. The relationship of these focus topics to TSPA-1995 and the NRC/CNWRA technical assessment program is illustrated in Figure 1-1. Each of these review topics was probed through the conjunctive use of simple and detailed process models, as well as through the use of the NRC Iterative Performance Assessment (IPA) Phase 2 computer code (Nuclear Regulatory Commission, 1995). These audit review analyses were documented in a manner that will permit DOE to understand NRC approaches that will be used in compliance determination.

As part of the second level review, the DOE TSPA methodology presented in TSPA-1995 was reviewed with respect to appropriateness of the technical approach (i.e., conceptual and mathematical models), treatment of uncertainties, use of conservative assumptions, sufficiency of site data, and consistency with previous DOE TSPAs.

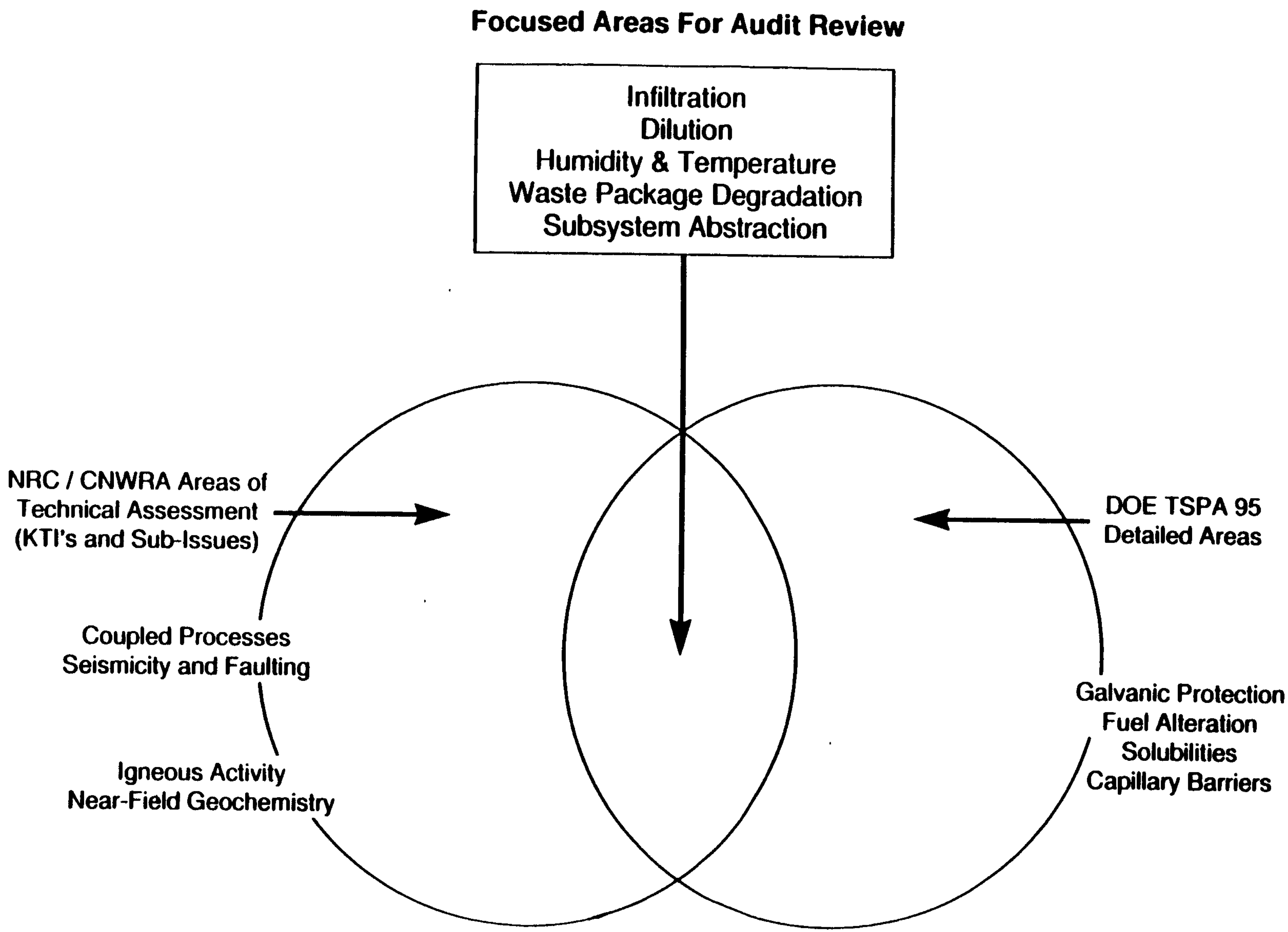

Figure 1-1. Selection of focus areas for audit review

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2 KEY TECHNICAL ISSUE: TOTAL SYSTEM PERFORMANCE ASSESSMENT AND TECHNICAL INTEGRATION

2.1 SCOPE OF REVIEW

The portions of TSPA-1995 relevant to the KTI concerning incorporation of relevant features, processes, events, uncertainties in parameters, selection of conceptual models, and prediction of future events into an analysis capable of estimating risk to an individual are identified in Table 2-1.

Table 2-1. Total System Performance Assessment 1995 scope of review for the Key Technical Issue: Total System Performance Assessment and Technical Integration

Section	Title
1.1	Background
1.2	Scope of the Current Total System Performance Assessment
1.3	Objectives of the Current TSPA
1.4	Analysis Components and Information Flow in the Current TSPA
1.5	Repository Integration Program (RIP)
1.6	Organization of the Current TSPA Document
8.1	Introduction
8.2	Major Assumptions and Key Parameter Values
8.3	Engineered Barrier System (EBS) Peak Release Rates
8.4	Cumulative EBS Release at 10,000 Years
8.5	Summary and Conclusions from EBS Performance Analyses
9.1	Introduction
9.2	10,000-Year Repository Performance
9.3	1,000,000-Year Repository Performance
10.1	Caveats
10.2	Significant Conclusions
10.3	Prioritization of Site Characterization and Design Activities
10.4	Summary of Conceptual Assumption Not Evaluated
10.5	Potential Impacts of Alternative Environmental Standards

Table 2-1. Total System Performance Assessment 1995 scope of review for the Key Technical Issue: Total System Performance Assessment and Technical Integration (cont'd)

Section	Title
10.6	Recommended Development, Substantiation, Documentation, and Testing of Process Level Models to be Used in Future TSPAs
10.7	Conservative and Nonconservative Factors Influencing the Predicted Results
10.8	Future TSPA Activities

2.2 AREA OF CONCERN: SUBSYSTEM ABSTRACTIONS

2.2.1 Description of the Total-System Performance Issue

Overall repository performance is presently quantified in terms of a complementary cumulative distribution function (CCDF) plot of total radionuclide releases (at 5 km) to the accessible environment (over 10^4 yr). DOE and NRC both utilize TSPA computer codes to assess repository performance. Previous CCDFs calculated by the DOE TSPA codes such as Total System Analyzer (TSA) [Wilson et al., 1994] and Repository Integration Program (RIP) [Golder Associates, Inc., 1993] have differed significantly from those computed by the NRC/CNWRA code, Total Performance Assessment (TPA) [Sagar and Janetzke, 1993]. These differences in calculational results are believed to be primarily due to distinct:

- Model abstractions of repository subsystems
- Parameter ranges and distributions
- Underlying and/or bounding assumptions

In Chapter 9 of TSPA-1995, a series of CCDFs computed with the RIP code are presented for various combinations of heat load, backfill, infiltration ranges, and alternative thermohydrologic models. None of these CCDF results are explained in terms of causal factors or basic performance indicators (e.g., residence time in the EBS, timing of condensate refluxing, particle travel times through the unsaturated and saturated zones). Thus, determining the correctness and reasonableness of the CCDF results requires independent calculation.

2.2.2 Description of Department of Energy Approach and/or Position

In the DOE TSPA-1995, the RIP computer code (Miller et al., 1992; Golder Associates, Inc., 1993) was used to estimate total releases of radionuclides to the accessible environment. These releases were then used to construct the CCDF for comparison with the total-system performance standards in 10 CFR 60.112. DOE selected RIP as its total-system performance computer code for various reasons. These include (TRW Environmental, 1995): (i) past experiences in the application of RIP to radioactive waste disposal systems in the United States and abroad, (ii) simplicity of its mathematical models, and (iii) computational efficiency.

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The RIP code consists of four main component models: (i) waste package behavior and radionuclide release from the engineer-barrier system, (ii) radionuclide transport pathways, (iii) disruptive events, and (iv) biosphere dose/risk. The component describing disruptive events, however, was not used in TSPA-1995. The RIP code requires a series of fixed and sampled input parameters for execution. In TSPA-1995, the many input parameters were obtained by conducting a limited set of calculations with process-level models to generate simple response-surface models. In addition, many assumptions and ad hoc procedures were used in selecting the parameter ranges and distributions. In TSPA-1995, often the assumptions used were not properly justified or supported by available data. For example, the fracture porosity in the unsaturated zone was assumed to be 0.001 for all strata, whereas for the saturated zone, a fracture porosity of 0.1 was assumed. No basis for assuming a larger porosity for the saturated zone was provided; moreover, the value selected is inconsistent with porosity values typical of fractured media.

2.2.3 Description of Nuclear Regulatory Commission Approach and/or Position

The NRC developed the TPA computer code for use in its review of critical aspects of the TSPAs to be submitted by DOE as part of its viability assessment and license application, and in the analysis of issues pertaining to overall performance. The TPA code was first used in the NRC IPA Phase 2 to compute the CCDF for cumulative releases (Nuclear Regulatory Commission, 1995).

TPA consists of: (i) an executive module; (ii) algorithms to develop vectors of uncertain input parameters by sampling from the respective statistical distributions; (iii) models that simulate future states or scenarios; and (iv) models that simulate internal repository system processes, such as the source term, and radionuclide transport in the geosphere and the biosphere (Sagar and Janetzke, 1993). The executive module controls the manner and sequence in which the modules containing the different models and algorithms within TPA are executed, and the transfer of data among modules within TPA. The TPA code as used in IPA Phase 2 consisted of the following modules, besides the executive module: AIRCOM, CLIMATO, CANT2, C14, DITTY, DRILL01, DRILL02, FLOWMOD, LHS, NEFTRAN, SEISMO, SOTEC, and VOLCANO (Nuclear Regulatory Commission, 1995). Of specific interest in these calculations is the SOTEC module. SOTEC calculated time- and space-dependent aqueous releases from the repository. However, as described below, the calculation of canister lifetime was bypassed in the module that was used in IPA Phase 2.

The approach used in the audit review calculations consisted of applying the IPA Phase 2 version of TPA in the following manner:

- Use a digitized canister lifetime CDF from TSPA-1995.
- Modify the TPA base-case data input file (used in IPA Phase 2) to represent TSPA-1995 data to the extent practicable.
- Calculate the CCDFs for radionuclide releases to the accessible environment for selected cases.
- Compare the TPA calculated CCDFs with the corresponding CCDF presented in TSPA-1995.

As in TSPA-1995, it was assumed that a canister failed when the wall was fully penetrated by the first pit. The canister lifetime history presented in Figure 5.7-10a of the TSPA-1995 report was

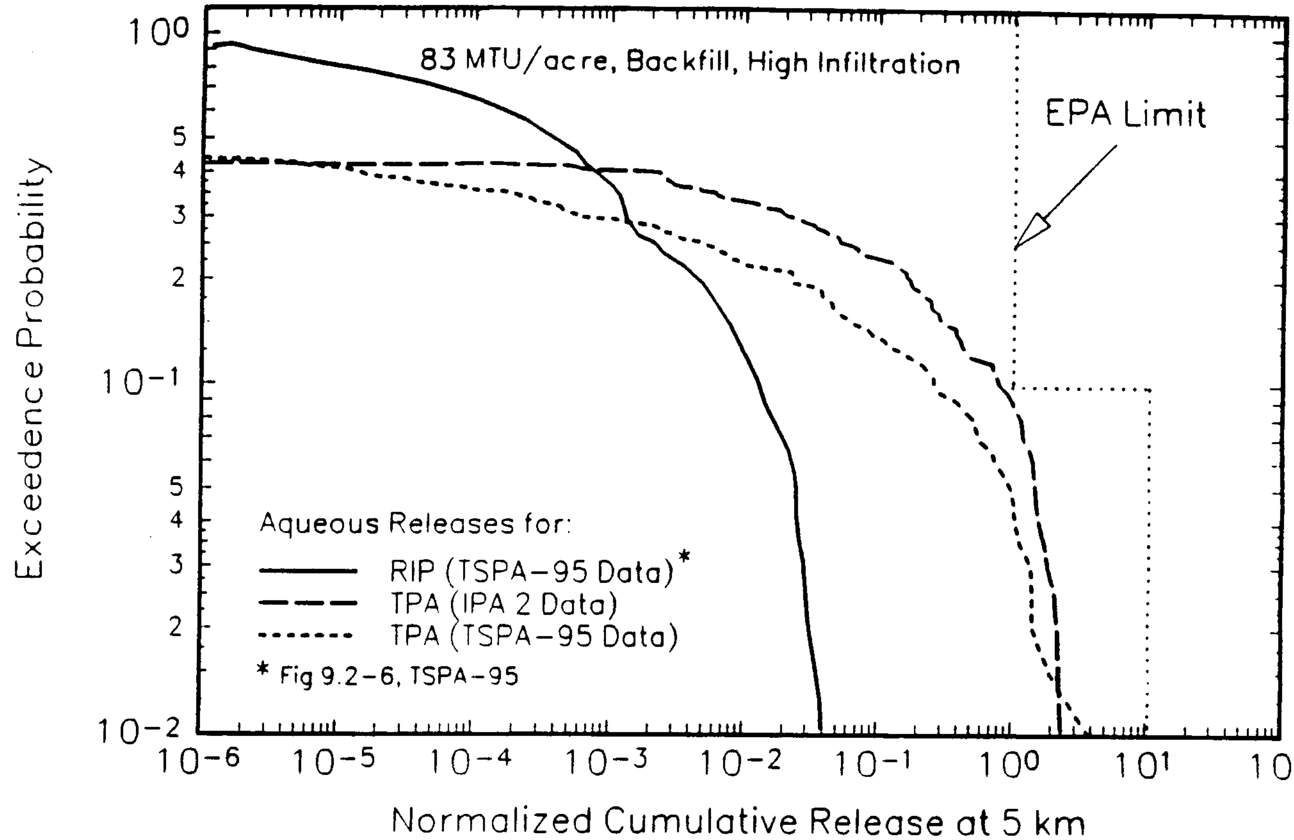

Figure 2-1. Comparison of complementary cumulative distribution functions for cumulative release

selected for this analysis. That figure gives the cumulative fraction of failures (by various corrosion processes) for various exposure times. This canister lifetime curve was calculated by RIP for the following canister conditions: thermal load of 82 MTU/acre, high infiltration, backfill, and RH-dependent corrosion initiation. The cumulative distribution function (CDF) in that figure was digitized and a histogram constructed. Two CCDFs independently computed with TPA are compared (see Figure 2-1) with the corresponding CCDF from TSPA-1995. The CCDFs generated by the TPA code utilized: (i) the original IPA Phase 2 data (unmodified) and the digitized TSPA-1995 canister lifetime curve, and (ii) the approximate representation of TSPA-1995 input data and the digitized canister lifetime curve.

In the first case, the CCDF calculated with TPA is close to the U.S. Environmental Protection Agency (EPA) limit whereas the CCDF taken from TSPA-1995 (i.e., calculated with RIP) is about two orders of magnitude below the EPA limit. The TPA calculations produced fewer lower releases and more higher releases than indicated by the TSPA-1995 result. This suggests that the IPA Phase 2 assumptions and site subsystem abstraction may be much more conservative than those used in RIP. Also, in the TPA calculations it was assumed that once a canister failed in a given zone of the repository, all canisters within that zone also failed, which is more conservative than the assumption used in TSPA-1995.

In the second case, the CCDF computed with the TPA again has fewer low releases and more higher releases than the CCDF produced by RIP in TSPA-1995. As in the first case, the TPA calculated CCDF differs significantly from that produced by the RIP code. The comparison suggests that, even when

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the data are similar, the abstracted models and conceptual representation of the system used in TPA are more conservative than those incorporated in RIP.

The major differences between the two independently calculated CCDFs and the selected CCDF from TSPA-1995 were hypothesized to be due to different:

- Methods for calculating particle travel times through the unsaturated zone
- Representations of the hydrostratigraphy of the unsaturated and saturated zones
- Discretizations of the repository foot print into subzones
- Assumptions regarding the canister failures in individual subzones

To evaluate the first of these hypotheses, the distributions of particle travel times were computed using the IPA 2 and RIP methods for particle travel time and a Monte Carlo sampling method. These calculations, performed with the MatLab software, produced CDFs for the particle travel time which are compared in Figure 2-2. As can be seen from this comparison, the CDF corresponding to the TPA model abstraction and data captures both fracture flow (i.e., fast pathways) and matrix flow behavior, whereas the RIP model abstraction and data lack an adequate representation of fracture flow.

In investigating the second hypothesis, the hydrostratigraphic models used in IPA 2 and TSPA-1995 were graphically compared (Figure 2-3). As can be seen from this comparison, the first six pathways (i.e., hydrostratigraphic columns that apply to the high heat load case) of the TSPA-1995 model are, in general, much longer than the IPA 2 subzone columns. In addition, the TSPA-1995 differs in that: (i) the Topopah Springs unit is subdivided into vitric (TSv) and welded (TSw) components and (ii) the Calico Hills nonwelded zeolitic (and low permeability) subunit is present in all of the TSPA-1995 pathways, in contrast to the IPA 2 model where it is absent in two of the seven columns. The longer path length and lower effective conductance of the flow path explains to a large degree the very long particle travel times computed in TSPA-1995. The absence of the short particle travel times or fast pathways in the TSPA-1995 are believed to be due to three aspects of the RIP particle travel time method: (i) matrix diffusion effect introduced by the Markovian method, (ii) formulation error in the calculation of the pore water velocity (i.e., Darcian flux should be divided by moisture content rather than effective porosity), and (iii) inadequate number of realizations in the process-level simulations used to estimate the effective ranges of matrix velocities and fraction of fracture flow.

The third hypothesis, regarding possible impact of different discretizations, is believed to explain the upper portion of the independently calculated CCDFs. The discretization used in the IPA 2 data set is irregular with some zones representing a large fraction of the repository area while others represent a very small fraction. In contrast, the discretization used in the TSPA-1995 data set is regular and apparently has equal areas. Thus, in the TPA calculations, the releases appear to have been dominated by one or two of the subzones with large areas. This irregular discretization, in combination with the assumption of one canister failure representing all canisters in the subzone (i.e., the fourth hypothesis), is believed to produce the high fraction of zero releases suggested in the independently calculated CCDFs.

While additional work is needed to fully delineate the factors producing the differences in the CCDFs, it should be noted that improvements in both the NRC and DOE approaches and data sets are needed. The DOE approach needs to better reflect the fast paths which are consistent with the

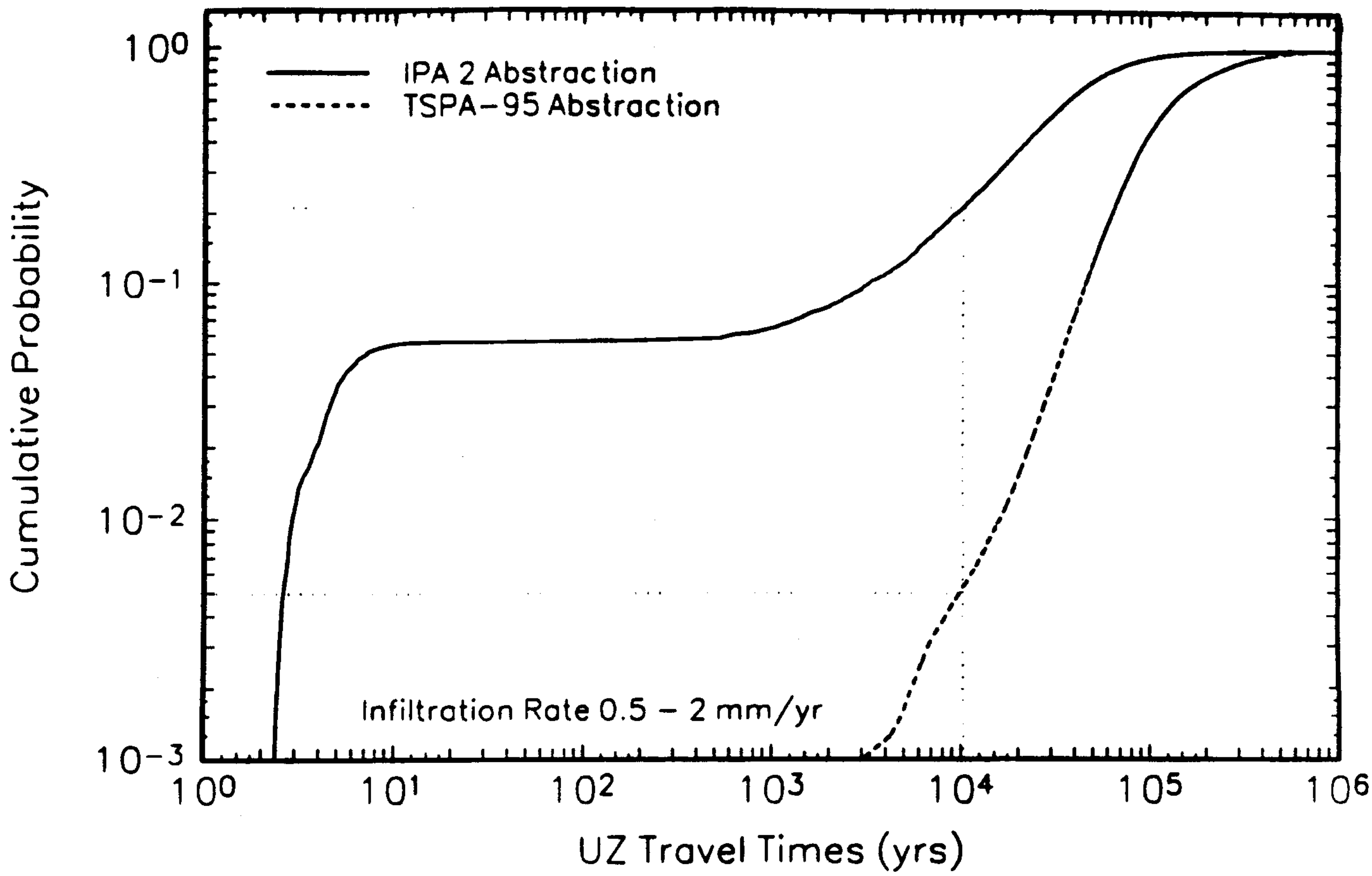
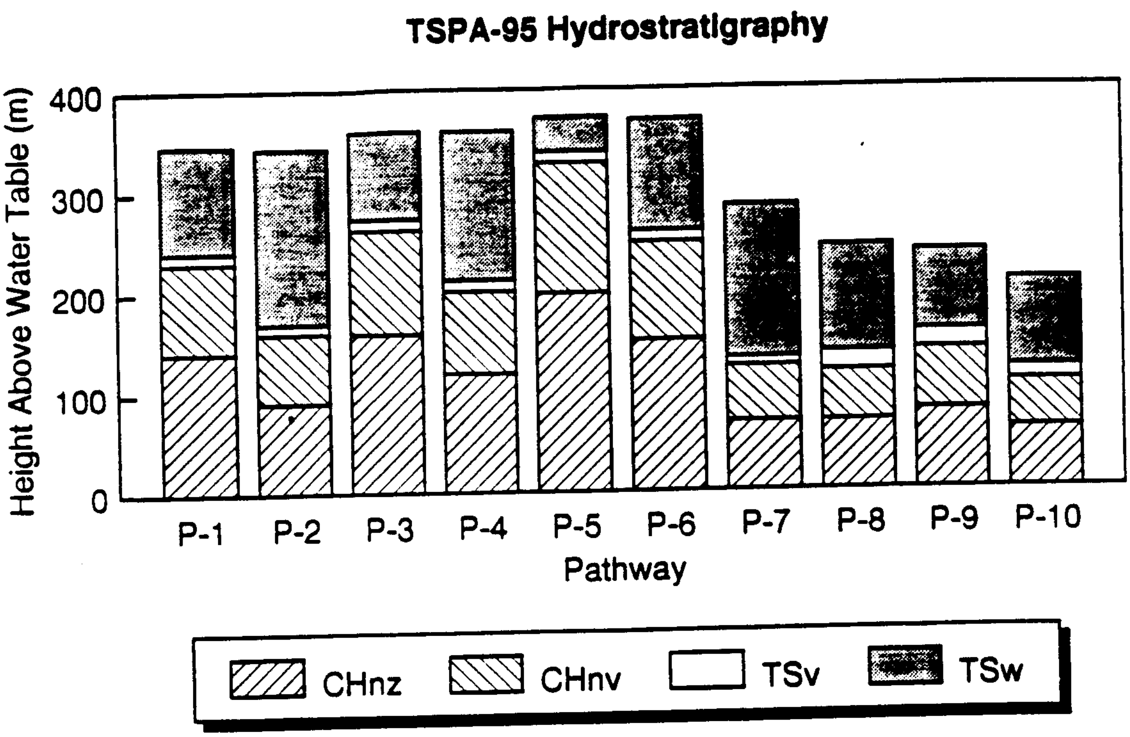


Figure 2-2. Comparison of particle travel-time cumulative distribution functions

hydrogeology of the YM site and with interpretations of recent chlorine-36 data (Fabryka-Martin et al., 1996). The NRC approach needs to utilize an updated representation of the hydrostratigraphy and regular discretization and to examine the possible over conservatism associated with the assumption of canister failures in repository subzones.



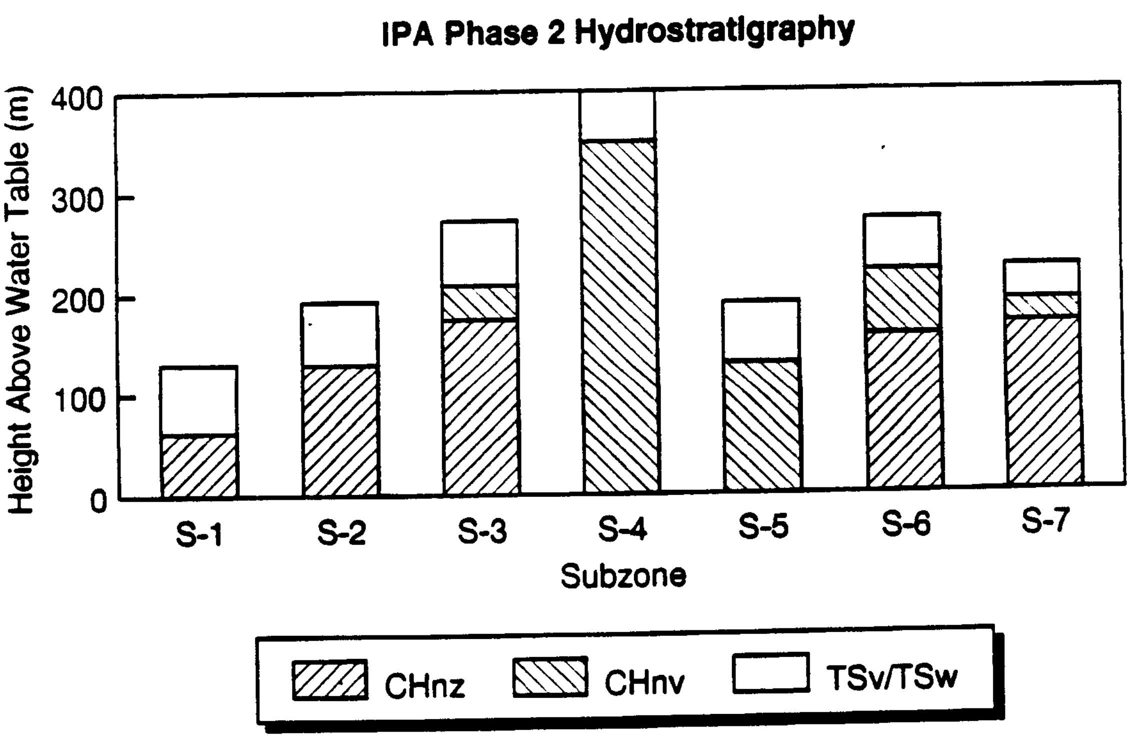


Figure 2-3. Comparison of hydrostratigraphic models

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3 KEY TECHNICAL ISSUE: IGNEOUS ACTIVITY

3.1 SCOPE OF REVIEW

The portion of TSPA-1995 relevant to the KTI concerning predicting the consequence and probability of igneous activity affecting the repository in relation to the overall system performance is identified in Table 3-1.

Table 3-1. Total System Performance Assessment 1995 scope of review for the Key Technical Issue: Igneous Activity

Section	Title
2.7.2	Igneous Activity

3.2 GENERAL COMMENTS—EXTERNALLY INITIATED IGNEOUS EVENTS AND PROCESSES

Statement of Concern: The conclusion that probability-weighted releases associated with igneous events and processes are insignificant is not based on analysis using parameters which agree with published data.

Basis of Concern: On Page 1–4, TSPA-1995 asserts that "the probability-weighted releases associated with externally initiated natural events and processes have been insignificant in comparison to the range in releases caused by repository-induced processes." This assertion is based on analysis reported on in Barnard et al. (1992) and Wilson et al. (1994).

The analysis in Barnard et al. (1992) for the direct effects of volcanic activity used a maximum eruptive volume of 1.0×10^8 m^3 of magma (see TSPA-1995, Figure 7-7). According to Crowe et al. (1995), Lathrop Wells had a magmatic eruptive volume of 1.4×10^8 m^3. Therefore, the maximum eruptive volume assumed in the calculations is less than the observed volume of the closest and youngest volcanic feature to the site. Estimated magma volumes for other Quaternary eruptions in the Yucca Mountain region (YMR) are 0.6×10^8 m^3 for Sleeping Butte and 2.3×10^8 m^3 for Crater Flat (Crowe et al., 1995).

The analysis in Barnard et al. (1992) assumed a mean value for wall-rock fraction of 0.03 percent and a maximum value of 0.06 percent (see TSPA-1995, Figure 7-8). According to Appendix F of Crowe et al. (1986), the average volume of material reported for Lathrop Wells nonhydromagmatic samples is approximately 1 percent. Samples that Crowe et al. (1986) considered as being of a hydromagmatic origin had values up to 17.5 percent. These values represent the data that has been documented by the DOE to date.

While other areas of the calculations could be questioned, use of the published Lathrop Wells values for these two factors would change the results of the Barnard et al. (1992) calculations significantly. In addition, the calculations fail to account for major differences between data collected from undisturbed geologic settings and the geologic setting that has been highly disturbed by the proposed repository, with regard to igneous processes and events.

In Wilson et al. (1994), the temperature in wall-rock adjacent to a cooling dike was calculated by an analytical formula for heat conduction in a semi-infinite composite medium. As has been pointed out in such places as Connor et al. (1996), the history of cooling and degassing from active basaltic analogs is strongly influenced by the thermo-physical properties of the rock and the degree of water saturation. For example, measurements taken at Tolbachik volcano in Kamchatka show that the area above a cooling dike is still in excess of 600 °C 20 yr after the eruptions. Fumarole temperatures at Jorullo volcano in Mexico are at 125 °C 220 yr after the eruption. The lack of correspondence between DOE models and observed cooling histories at active volcanos raises questions concerning both the models and the results produced with them.

The staff notes that, on Page 2-11 of TSPA-1995, DOE was advised that release calculations will need to include estimates for eruptive releases.

Recommendation: Future calculations which consider the effect of igneous disruptive processes need to include parameters which most accurately portray or bound the documented effects of igneous processes.

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4 KEY TECHNICAL ISSUE: UNSATURATED AND SATURATED FLOW UNDER ISOTHERMAL CONDITIONS

4.1 SCOPE OF REVIEW

The portions of TSPA-1995 relevant to the KTI concerning the characterization of unsaturated and saturated flow (liquid and vapor phase) at YM under ambient thermal conditions are identified in Table 4-1.

Table 4-1. Total System Performance Assessment 1995 scope of review for the Key Technical Issue: Unsaturated and Saturated Flow under Isothermal Conditions

Section	Title
2.1	Introduction
2.2	Geo-environmental Framework
2.3	Hydrostratigraphy
2.4	Matrix/Fracture Hydrogeologic Properties
2.5	Regional Hydrology and Groundwater Use
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4.2 AREA OF CONCERN: INFILTRATION

4.2.1 Description of the Total-System Performance Issue

The distribution of percolation flux is identified in TSPA-1995 (TRW Environmental Systems, Inc., 1995, Chapter 10) as the primary site characterization issue, due to impacts on WP degradation and radionuclide transport rates through the unsaturated zone. Infiltration rates are assumed to control percolation fluxes. The two concepts can be used synonymously when flow in the unsaturated zone is essentially steady state and vertical, so that vertical percolation flux is the same at every depth.

Infiltration and deep percolation calculations presented in Chapter 7 of TSPA-1995 lack defensibility because of:

- Unsupported assumptions made in abstracting process-level matrix and fracture flow velocities, and a flow partitioning factor, into probability density functions (PDFs)
- Incorrect equation for fracture-flow velocities
- Poor correspondence between the statistical behavior of process-level calculations and abstracted calculations

The degree of conservatism incorporated in the infiltration and deep percolation calculations presented in TSPA-1995 is presently unclear.

4.2.2 Description of the Department of Energy Approach and/or Position

In the DOE TSPA-1995, percolation fluxes are used for two purposes: (i) estimation of radionuclide transport rates in the natural barrier system (the "mountain-scale" model), and (ii) estimation of WP corrosion rates and radionuclide release rates (the "drift-scale" model). Both models use areal-averaged infiltration rates as the direct estimator for deep percolation fluxes in both the matrix and in an assumed fracture continuum. Variation of infiltration rate due to changes in climatic is computed by multiplying the base infiltration rate with a sawtooth function that is one at present time, increases to a randomly selected maximum at 50,000 yr in the future, returns to one at 100,000 yr in the future, and repeats until the end of the simulation.

At the mountain scale, flow is assumed to be essentially 1D in the vertical direction, and each stratigraphic layer is assumed to be homogeneous. The response of the liquid velocity in each stratigraphic layer and the fraction of flow in the fracture continuum for each layer is constructed as a function of the areal-average infiltration flux. Fracture properties do not vary between layers nor between realizations. For each of six infiltration fluxes, a 1D column with a representative stratigraphy, one of ten matrix-property realizations, and one of two fracture-flow-initiation models, is used to estimate both the velocity in the matrix and the fraction of flow in the fractures. A maximum and minimum value for each layer are extracted for both estimated properties at each infiltration rate. During transport simulations, a value for the infiltration rate is randomly selected and the corresponding maxima and minima for each layer are obtained from the previous calculations. The fracture-flow-fraction value used in the transport simulation is assumed to be uniformly distributed between the maximum and minimum values, while the matrix-velocity value is log-uniformly distributed.

At the drift scale, the response of the expected dripping flux and the expected fraction of the WPs contacted by a drip is constructed as a function of the areal-average infiltration flux. For each of ten values of areal-average infiltration flux, assumed probability distributions for the drift-scale deviation of infiltration rates about the areal-average rate and drift-scale values of saturated hydraulic conductivity are used to calculate both the expected dripping flux and the expected waste-package-contact fraction. These expected values are used for calculations of waste-package corrosion and drift-scale transport. It is assumed that the fraction of packages contacted by drips remains constant under climatic variation, although the drip flux is allowed to vary.

4.2.3 Description of the Nuclear Regulatory Commission Approach and/or Position

The NRC endorses the use of the DOE hierarchical PA approach articulated in DOE TSPA-1993 (Wilson et al., 1994). Applying that approach to infiltration rates, percolation fluxes, and fluid velocities would suggest the conjunctive use of simple models such as those described in the DOE TSPA-1995 and more detailed process models. However, the application of the models should use the probabilistic description of the hydraulic parameters to derive a self-consistent probabilistic description of the resultant percolation fluxes.

In order to estimate deep percolation fluxes at and below the proposed repository over geologic time, a linkage between climatic influences and deep percolation is necessary. In the TSPA-1995 report, it is assumed that climatic variation can be described using a 100 ka sawtooth function. The approach plausibly provides 10 glacial cycles within a period of 1 Ma, although the assumption that there is a chance that no increase in infiltration flux occurs under glacial conditions does not seem reasonable. As it currently stands, however, the period of regulatory interest is 10 ka, so that it is not clear that the TSPA-1995 approach is conservative. Based on evidence ranging from measurements of ice caps, calcite veins, and sea-floor sediments (Winograd et al., 1988; 1992), climatic variation can also occur over considerably shorter time scales. Due to the sensitive dependence of releases to infiltration rates, accommodating the full range of climatic variation possible within the current 10 ka regulatory period would be more conservative.

Fluxes and velocities in the matrix and fractures are not directly calculated in the total-system simulations reported in TSPA-1995. Rather, an abstracted representation for these quantities is used. Using a single representative vertical column with constant thicknesses, random matrix properties obtained from Schenker et al. (1995) [essentially identical to the properties used in the TSPA-93 report Wilson, et al., (1994)], and a single set of constant fracture properties for all stratigraphic layers, the velocities and fluxes obtained from simulations using TOUGH2 (Pruess, 1987; 1991) for a small number of material-property realizations are abstracted into PDFs for matrix velocity (V_m), fracture velocity (V_f), and a flux-partitioning factor (F_f) distributing flux between matrix and fractures.

There are a number of components of the abstraction process that do not build confidence in the conservatism of the abstracted model. These components include:

- The equivalent-continuum conceptual model is different than flow models used in previous TSPA analyses, and no comparison between models is made.
- The equivalent-continuum conceptual model has an arbitrary satiation parameter, σ, that cannot be measured.
- The underlying form of the PDFs describing V_m, V_f, and F_f is assumed without justification.
- The parameters describing the PDFs for V_m, V_f, and F_f are estimated from the minimum and maximum observed values for V_m and F_f. It is doubtful that the extremum values resulting from the underlying PDFs would occur with the rather limited set of ten material-property realizations. It is questionable whether the mean behavior of V_m, V_f, and F_f would be captured from even the true extremum values.

- The transport velocity in fractures incorrectly assumes that the fractures are completely saturated, thereby underpredicting the velocity in fractures. Based on the saturated hydraulic conductivity for the fracture continuum, one would expect that velocities are underpredicted by at least one to two orders of magnitude.

- Available information regarding material-property PDFs is not incorporated into the abstraction. In particular, Schenker et al. (1995) provide correlations between porosity and permeability, and provide information on fracture properties.

On the other hand, the implementation of the abstraction process may be conservative insofar as it is guaranteed that there is some flux from the repository directly to the water table in fractures, for essentially every realization, even though this may not be the case for the process-level simulations that the abstraction is based on. However, it is not guaranteed that higher mean levels of flux occur in fractures for the abstractions.

In order to independently assess the impact of the assumptions used for the abstraction, the process presented in the TSPA-1995 report was followed for several flux rates. The fairest test would be to compare contaminant releases using process-level simulations with the corresponding contaminant releases using the abstraction. Unfortunately, it is impossible to reproduce the transport simulator based on information provided in the TSPA-1995 report. Accordingly, a surrogate measure was adopted for the following analysis. The surrogate measure is nondecaying-particle travel time through each pathway in the 1D column, where a pathway consists of a combination of matrix flow for some layers and fracture flow for the remaining layers. For example, the fastest pathway would typically consist of fracture flow for each of the four layers, and the slowest pathway typically consists of matrix flow through each layer. Particles do not switch between matrix and fracture within a layer but may at layer interfaces. The 12 curves presented in Figures 4-1 and 4-2 represent a matrix, where the line style (dotted, solid, dash-dot) represents the pathway and the symbol style denotes procedure used to generate the pathways. Three pathways are of particular interest: (i) the fastest pathway, (ii) the slowest pathway, and (iii) the pathway with the largest flux.

The two extreme flux rates considered in the TSPA-1995 abstraction process, 2 mm/yr and 0.01 mm/yr, are considered in Figures 4-1 and 4-2, respectively. These figures examine the fastest, slowest, and largest-flux pathways for each of 50 process-level realizations, and corresponding pathways using the abstractions from the 50 process-level realizations. The cumulative fraction of realizations with the particle travel time for a specified pathway not exceeding a given particle travel time is presented for each pathway. As a comparison, the corresponding pathway analysis is performed for the TSPA-1995 abstraction. The process-level simulations were performed by integrating Darcy's law from the water table to the repository, using the steady-state ordinary differential equation-solver approach described by Baca et al. (1994) adapted to incorporate the equivalent continuum model used in the TSPA-1995 abstraction.

Examining the behavior of the 2 mm/yr case in Figure 4-1, it can be seen that the statistical behavior of the particle travel times for the process-level pathways is somewhat different from the behavior of the corresponding abstraction pathways. In particular, the process-level simulations exhibit a relatively low but non-negligible probability of extremely fast pathways, on the order of decades, while the largest-flux pathways and most of the fastest pathways are on the order of 10^4 yr. Incorporating a total of 320 simulations (not shown here due to space limitations) suggests that there is a small probability that the largest-flux pathways may also be on the order of decades. On the other hand, the abstraction from these process-level simulations has fastest pathways at least 200 yr, usually on the order of 1,000 yr;

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largest-flux pathways generally tend to be several times slower than the corresponding process-level simulations. By comparing the 50-realization abstraction with the TSPA-1995 abstraction, it can also be seen that considering 50 material-property realizations, rather than ten realizations, has the effect of making the fastest pathways faster and the slowest pathways slower.

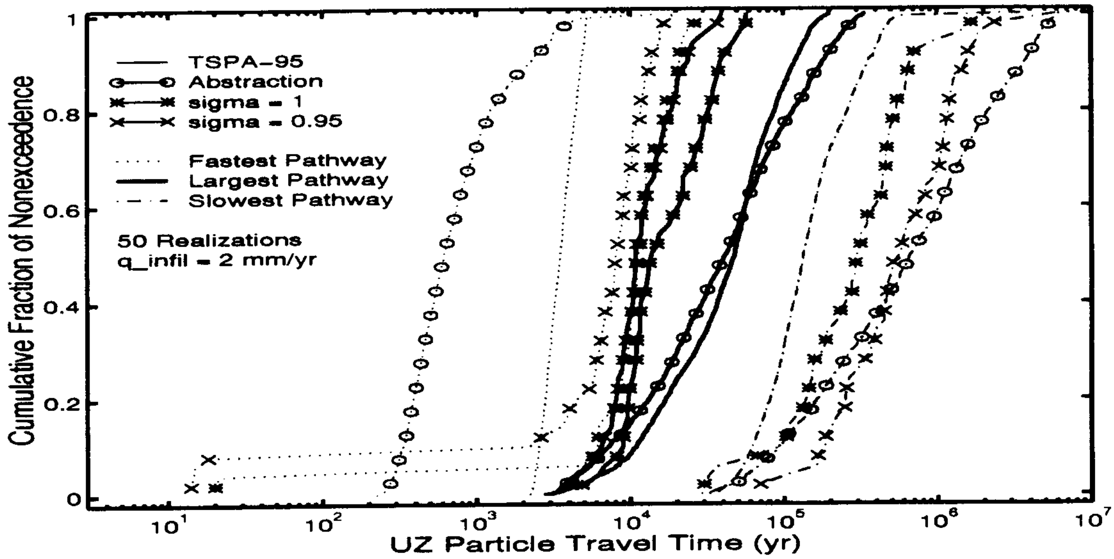

Figure 4-1. Comparison of process-level simulations with abstractions for an infiltration flux of 2 mm/yr

Examining the behavior of the 0.01 mm/yr case in Figure 4-2, the abstraction can be seen to have a drastic impact on the spread of particle travel times, but does not strongly affect the largest-flux pathways. It is not clear whether an artificial spread in travel times means the abstraction is conservative. Admittedly, the very low velocities would yield no releases in 10^4 yr.

The infiltration fluxes used in the total-system simulations are based on infiltration estimates by Flint and Flint (1994), which in turn are based on measurements of the saturated hydraulic conductivity of outcrop units. Since the TSPA-1995 simulations were performed, Flint et al. (1995) have provided new estimates for shallow infiltration that are several orders of magnitude larger over the repository footprint than the Flint and Flint (1994) estimates. The new estimates are based on measurements of infiltration in a network of 70 to 100 neutron-probe boreholes. Taking into consideration recent measurements of elevated levels of chlorine-36 in the Exploratory Studies Facility (ESF) (Fabryka-Martin et al., 1996), it appears difficult to justify deep percolation rates that consistently yield fastest-pathway particle travel times from the repository to the water table that are in excess of decades to centuries. Accordingly, the combination of extremely small deep-percolation fluxes (e.g., 0.01 mm/yr) with an equivalent-continuum model does not appear to provide a reasonably conservative bound on the behavior of deep percolation in the face of the latest field evidence.

The latest field evidence also suggests that shallow infiltration may not be distributed uniformly over the subregional area. If indeed this is the case, the effect on deep percolation past the repository may be significant. Preliminary 2D vertical-slice simulations using BIGFLOW (Ababou and Bagtzoglou, 1993),

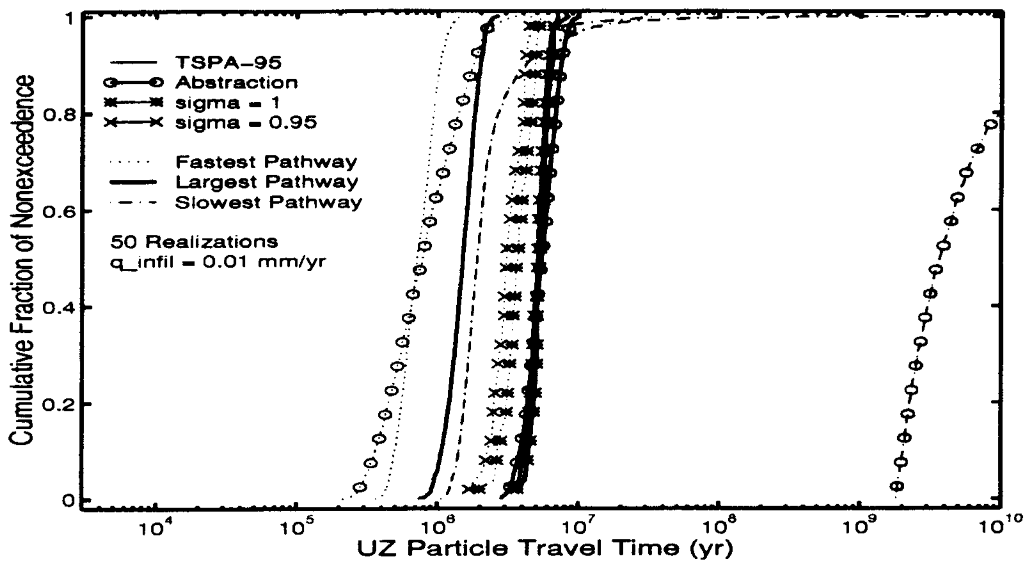

Figure 4-2. Comparison of process-level simulations with abstractions for an infiltration flux of 0.01 mm/yr

assuming matrix-only flow, suggest that focused infiltration can have a significant impact on fluxes past the repository. This point is demonstrated in Figure 4-3, which shows the impact that localizing infiltration has on fluxes past the repository. Two east-west cross-sections are considered, crossing the northernmost and southernmost portions of the repository footprint, with two and three simulations, respectively [for details see Bagtzoglou et al., (1995)]. The horizontal axis represents the distributed flux that is equivalent to spreading the localized infiltration over the entire ground surface such that an identical amount of water enters the system. The vertical axis represents the flux in the individual elements corresponding to the repository, normalized by the distributed flux. Despite admitted limitations in the approach, the figure clearly suggests that focusing shallow infiltration can significantly increase or decrease the flux past the repository. Thus, it is not clear whether it is conservative to neglect focused recharge and subsequent lateral flow as is done in the TSPA-1995 report.

In summary, the TSPA-1995 report presents a method for abstracting PDFs that describe the velocities and fluxes obtained from a set of detailed process-level simulations. The presentation of the abstraction procedure suffers from significant omissions and errors, thereby greatly weakening confidence in the reported results. However, the magnitude of the uncertainty in assigning the deep percolation rate to a process-level simulation may outweigh the persistent errors in abstracting the results of the process-level simulations.

4.2.4 Description of Likely Effects on Performance

Infiltration rates and percolation fluxes impact the performance of the proposed YM repository in two primary ways: (i) facilitation of WP degradation, and (ii) transport of radionuclides from the repository to the water table. Accordingly, infiltration rates are consistently found to strongly impact performance assessments of the proposed YM repository. Therefore, infiltration rates will play a central role in determining compliance with the expected risk- or dose-based standard.

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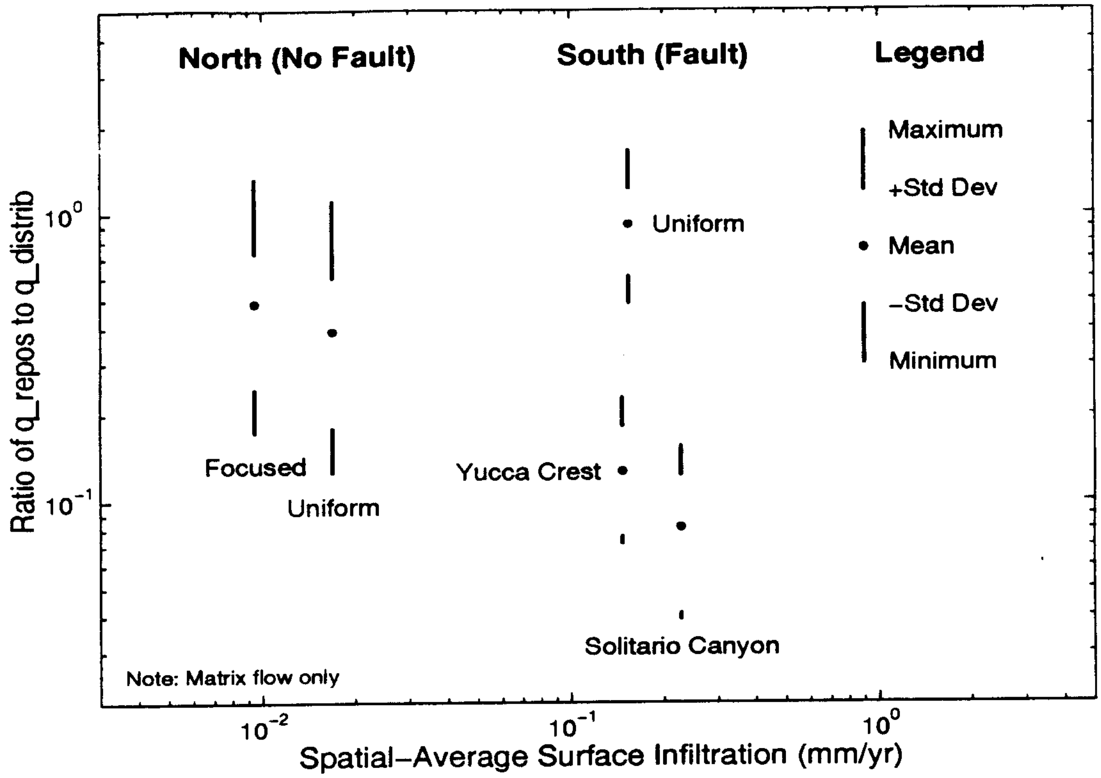

Figure 4-3. Statistical description of element fluxes at the repository level, normalized by equivalent uniform infiltration flux applied at the ground surface for two east-west cross-sections and three focusing strategies

In developing its safety case for YM, the DOE is currently conducting a detailed and thorough evaluation of infiltration rates and the resulting deep percolation rates, through a combination of activities including computer modeling (abstracted and detailed), evaluation of field-measured infiltration rates, measurement of field- and laboratory-scale hydraulic properties for both matrix and fractures, and incorporation of measured properties in their computer models. This data and information is expected to strengthen the defensibility of future TSPAs.

4.3 AREA OF CONCERN: DILUTION

4.3.1 Description of the Total-System Performance Issue

Groundwater dilution at the YM site could have several orders of magnitude impact on total-system performance relative to a dose- or risk-based compliance standard. Consequently, the estimation of dilution merits a combination of: (i) detailed site scale (e.g., 5 km) and regional scale (e.g., 30 km) groundwater modeling, (ii) evaluation of geochemical parameters indicating the degree of mixing, and (iii) estimation of macro-scale dispersivities based on field tracer test data. Such a combination of investigations would better support DOE developing a defensible basis for the site viability assessment.

Dilution factor calculations presented in Chapter 7 of TSPA-1995 (pp. 7-22 through 7-26) lack defensibility because of:

- Inappropriateness of conceptual models implicit in the analytical models utilized
- Failure to use available hydrologic, geologic, and geochemical field data in the analysis
- Possible misinterpretation of existing groundwater budget data

The dilution calculations presented in TSPA-1995 do not make use of (or build upon) previous DOE site scale flow and transport analyses conducted for TSPA-1993 (Wilson et al., 1994) or regional groundwater flow analyses conducted by the USGS (Czarnecki and Waddell, 1984).

4.3.2 Description of the Department of Energy Approach and/or Position

In TSPA-1995, two models are used to estimate dilution factors: a "stirred tank" mixing model and a line source "advection-dispersion" model. The stirred tank model implicitly assumes that radionuclides leaving the repository are uniformly distributed over the entire repository footprint and, upon reaching the water table, are instantaneously and completely mixed over a 50 m thick zone (i.e., screen-interval depth). In contrast, the advection-dispersion model makes no assumption of mixing depth but rather assumes the radionuclides enter the saturated zone along a line equal to the width of the repository (e.g., 4 km) and that macro-scale dispersion reduces concentrations along the flow path from the repository to Amargosa Desert.

Based on the stirred tank model, TSPA-1995 calculates dilution factors ranging from 8×10^2 to 3.3×10^4 for a 5 km path length. With the advection-dispersion model, TSPA-1995 estimates centerline dilution factors of 4.5×10^3 to 1.9×10^5 for a 5 km path length and 3.1×10^4 to 1.3×10^6 for 30 km. Embedded in the calculations with the advection-dispersion model is the assumption that dispersion coefficients are linearly dependent on path length. The range of groundwater fluxes used in the dilution calculations are based on information from undocumented flow modeling.

4.3.3 Description of the Nuclear Regulatory Commission Approach and/or Position

The NRC endorses the use of the DOE hierarchical PA approach articulated in the DOE TSPA-1993 (Wilson et al., 1994). Applying that approach to dilution would suggest the conjunctive use of simple models such as those described in TSPA-1995 and more detailed process models such as those used in TSPA-1993. However, the application of the stirred tank and advection-dispersion model should utilize conceptual models and model parameters consistent with available site hydrologic and geologic field data. In addition, the reasonableness of these calculations should be confirmed with available geochemical data.

Stirred Tank Model: In applying the stirred tank model, the analysis assumes uniform flow across a 50 m screened-interval depth. However, the stirred tank model is applicable to only natural mixing and not mixing induced by pumping. Thus, the use of a screened-interval depth is not appropriate. Moreover, this model applies to a specified volume of water beneath the repository and not to a 5 km path length as asserted in TSPA-1995 (pp. 7-25).

Available hydrogeologic data indicate that the groundwater beneath the proposed site is predominantly moving along thin fracture zones which is evident from borehole flow survey data for UE-25b #1 (Lobmeyer, et al., 1983; Lahoud, et al., 1984) as well as for UE-25c #1, #2, and #3 (Geldon, 1993). The localized nature of the flow is apparent from the data presented in TSPA-1995 Figure 4-4, which is taken from the report of Geldon (1993). Therefore, a more appropriate conceptualization is a plume confined to a single fracture zone near the water table with the thickness of the zone estimated from field data. Available data suggests that fracture zone thicknesses are typically smaller than the 50 m mixing depth assumed in the TSPA-1995 calculation.

The TSPA-1995 dilution calculations utilize an average saturated zone flux of 2 m/yr which was taken from an incompletely referenced modeling study conducted by Sandia National Laboratory (cited as Barr, 1993). However, groundwater fluxes can be estimated directly from available head data and hydraulic conductivity data. For example, available potentiometric-surface maps (Robison, 1984; Ervin, et al., 1993; Wittwer et al., 1995) suggest a head gradient across the repository of about 3×10^{-4}, although significantly larger hydraulic gradients occur to the west and north of the repository [0.015 and 0.15, respectively (Fridrich et al., 1994)]. Similarly, hydraulic conductivities determined from pump tests for borehole UE-25b#1 (Lahoud et al., 1984) for fracture zones range from 10^{-1} to 1 m/day. These hydraulic conductivities convert to 1.2×10^{-6} m/s (36.5 m/yr) and 1.2×10^{-5} m/s (365 m/yr), respectively.

Utilizing the UE-26b#1 conductivities and a mean hydraulic gradient of 3×10^{-4} the saturated zone fluxes (q_{SZ}) calculated from Darcy's law fall in the range of 0.01 to 0.1 m/yr. Assuming a 10 m fracture zone, the stirred tank model (TSPA-1995, pp. 7-25) for the dilution factor (DF) simplifies to:

$$DF = \frac{q_{SZ}}{q_{UZ}}\frac{W_{Rep}h}{A_{Rep}} = \frac{q_{SZ}}{q_{UZ}}\frac{4000m\times10m}{4\times10^5m^2} = \frac{q_{SZ}}{q_{UZ}}\times0.1 \qquad (4\text{-}1)$$

where q_{UZ} is unsaturated zone flux (m/yr), W_{Rep} is the width of the repository (m), A_{Rep} is the area of the repository (m^2), and h is the depth of the fracture zone (m). Using the estimated groundwater flux of 0.1 m/yr and q_{UZ} values (1.25×10^{-3} and 3×10^{-5} m/yr) cited in TSPA-1995, the above equation yields a range of dilution factors of 8.0 to 333.3, which are 2 orders of magnitude smaller than those reported in the TSPA-1995. Utilizing the maximum q_{UZ} values from the NRC Iterative Performance Assessment (IPA) Phase 2 (Nuclear Regulatory Commission, 1995) for the dry and pluvial conditions, one computes a range of dilution factors of one to two.

Advection-Dispersion Model: In applying the advection-dispersion model, the TSPA-1995 assumes a constant groundwater flux of 2 m/yr and transverse dispersivities of 30 m. The steady-state analytical solution for the advection-dispersion model yields the expression for dilution factor (TSPA-1995, pp. 7–25)

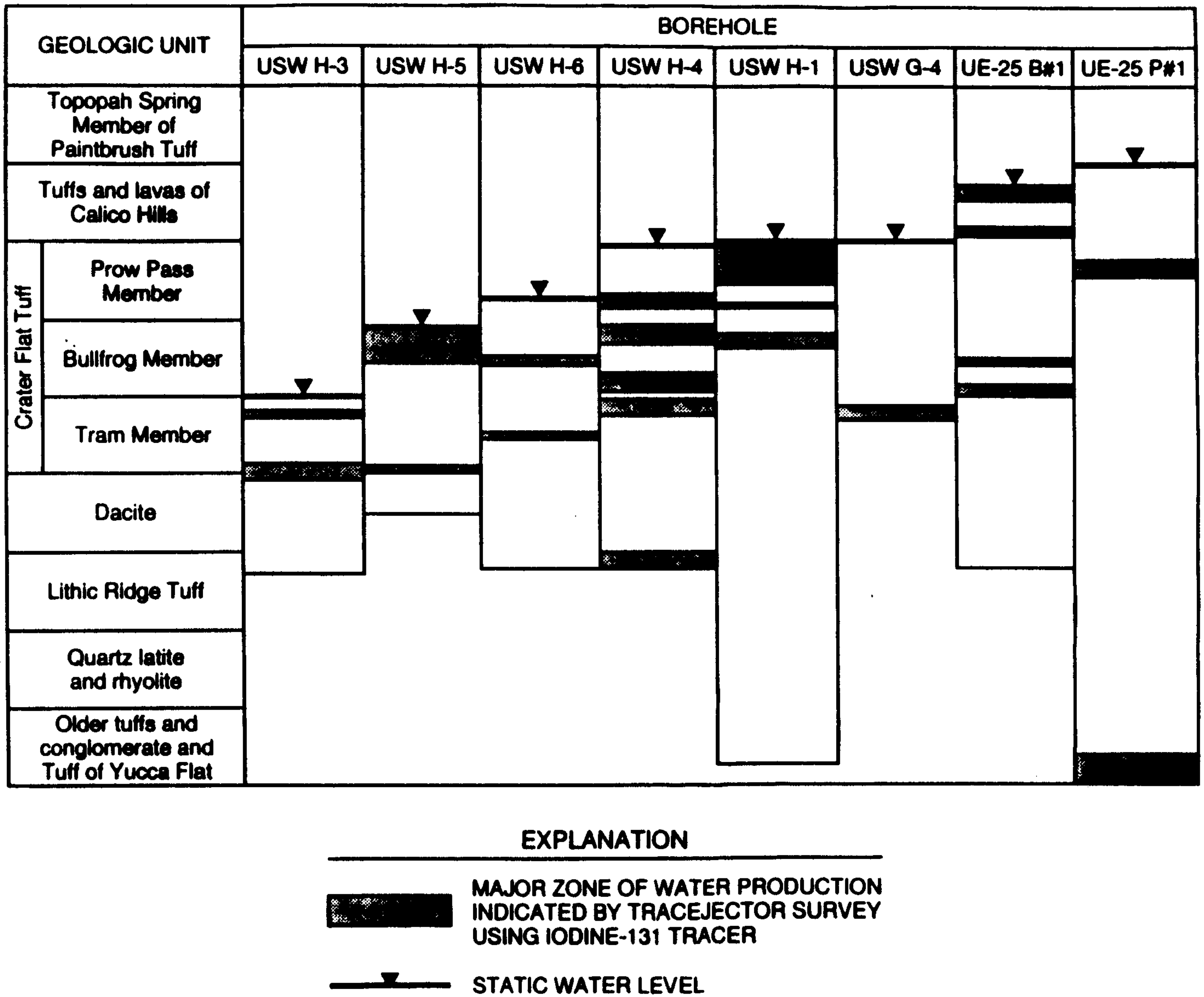

Figure 4-4. Major water-production zones in Tertiary rocks and static water levels in boreholes drilled at Yucca Mountain (taken from Geldon, 1993)

$$DF = \frac{q_{sz}}{q_{uz}} \frac{l}{A_{rep}} \frac{\sqrt{\pi \alpha_T x}}{erf\left\{\frac{l}{4\sqrt{\alpha_T x}}\right\}} \tag{4-2}$$

where α_T is the transverse dispersivity and l is the length of the line source (equal to the width of the repository). This analytical solution is written explicitly in terms of the transverse dispersivity (assumed uniform in the y- and z-directions), rather than the dispersivity-scale coefficients used in TSPA-1995. Transverse dispersivity is typically estimated to be about 1/5 to 1/100 of the longitudinal dispersivity α_L (de Marsily, 1986). Standard practice for estimating longitudinal dispersivities is to take α_L as 1/10 of the path length (Fetter, 1993). Using this rule of thumb and assuming α_T/α_L=1/50, conservative estimates are α_T=10 m for 5 km and α_T=60 m for 30 km flow paths.

The groundwater flux for the 5 km path length is taken as 0.1 m/yr which was previously estimated from available field data. For the 30 km path length, the groundwater flux can be estimated from available potentiometric-surface maps and an estimate of hydraulic conductivity. In the vicinity of the Amargosa Valley, the hydraulic head gradient appears to be about 10^{-3} or less. From the modeling study of Czarnecki (1985) for the regional groundwater system, the hydraulic conductivity in the alluvium is estimated to be about 1.7×10^{-5} m/s. These estimated hydraulic properties lead to an estimate of regional groundwater flux of about 0.5 m/yr.

Using the above values and TSPA-1995 values for q_{UZ}, dilution factors calculated with Eq. (4-2) are summarized in Table 4-2.

Table 4-2. Dilution factors computed using Department of Energy q_{uz} values with conservative q_{sz} and α_T

q_{uz} (m/yr)	Dilution Factor (DF)	
	5 km	30 km
1.25×10^{-3}	9.5×10^{2}	8.0×10^{3}
3.0×10^{-5}	4.0×10^{4}	3.4×10^{5}

These calculated dilution factors are about 1/3 to 1/5 of those estimated in TSPA-1995. Utilizing the maximum q_{UZ} values from the NRC IPA Phase 2 (NRC, 1995), the following dilution factors are calculated, which are presented in Table 4-3. For these assumptions, the dilution factors are about 2 to 3 orders of magnitudes smaller than those calculated in TSPA-1995.

Table 4-3. Dilution factors computed using Nuclear Regulatory Commission Iterative Performance Assessment Phase 2 q_{uz} values with conservative q_{sz} and α_T

q_{uz} (m/yr)	Dilution Factor (DF)	
	5 km	30 km
1.0×10^{-2}	1.2×10^{2}	2.0×10^{3}
5.0×10^{-3}	2.4×10^{2}	3.4×10^{3}

Based on the groundwater budget data in Table 2.5-1 of TSPA-1995, it appears that the dilution factor for the groundwater withdrawal zone should be 2.5 rather than 3.5 as cited in Section 7.6.3 of TSPA-1995. The value of 2.5 is arrived at by dividing the total inflow to the Amargosa Desert (20,000 ac-ft/yr) by the outflow from Jackass Flat/Buckboard Mesa (8,000 ac-ft/yr), which is influent to the Amargosa Desert. Apparently in TSPA-1995 it was assumed that the 20,000 ac-ft of annual inflow to the Amargosa Desert does not already include the 8,000 ac-ft influent from Jackass Flat/Buckboard Mesa.

A recent evaluation (Wittmeyer and Turner, 1996) of hydrochemical data from boreholes in the Amargosa Desert indicates that recognizable hydrochemical tracer signatures of different recharge sources, particularly for stable isotopes such as deuterium and ^{18}O, are preserved over distances on the order of tens of kilometers. Moreover, analyses of aqueous carbonate chemistry and calcite saturation in the fractured tuff aquifer by Murphy (1995) provide support for channeling of flow within the saturated zone. The general heterogeneity of hydrochemistry in the YM region and persistent hydrochemical signatures in the Amargosa Desert region indicate that regional flow is more complex than the stirred tank conceptual models used in TSPA-1995 to account for dilution immediately below the repository and in the groundwater withdrawal area. This evidence also suggests that actual mixing and dilution that occurs in the YM and the groundwater withdrawal areas may be less than assumed in TSPA-1995.

4.3.4 Description of Likely Effects on Performance

Dilution of contaminants in the groundwater will occur as a result of natural mixing and mixing induced by groundwater withdrawal. Dilution is an important factor in the assessment of performance because it determines the degree of dose reduction. Therefore, dilution will play a central role in determining compliance with the expected risk- or dose-based standard.

In developing its safety case for YM, the DOE should strive to make a detailed and thorough evaluation of groundwater mixing and dilution effects through a combination of activities including computer modeling (abstracted and detailed), evaluation of geochemical parameters, and field tracer testing. Alternatively, the DOE may choose to develop a conservative bound for dilution effects.

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4.4 GENERAL COMMENTS—MATRIX SATURATION

Statement of Concern: The degree of matrix saturation at which fracture flow is initiated is a critical choice for the TSPA calculations. In TSPA-1995, it is recognized that the conventional formulation requiring full saturation of the matrix prior to the initiation of fracture flow (Tsang and Pruess, 1989) arbitrarily reduces the occurrence of modeled fracture flow at YM. In an attempt to add more realism, calculations in TSPA-1995 consider a "relaxation" of this requirement so that fracture flow may begin when the matrix reaches a "satiated matrix saturation." Such an addition of realism and conservatism to the calculations is desirable; however, the lower limit chosen for the "satiated matrix saturation" remains unrealistically high and inadequately conservative.

Basis of Concern: The limits chosen for this "satiated matrix saturation" are 1.0 to 0.95. The lower limit is claimed to be justified because "numerical experiments with (satiated matrix saturation) values less than 0.95 appear to result in an exaggeration of fracture flow" (TSPA-1995, pp. 7-7 and 7-8). Xiang et al. (1995) note that the equivalent continuum model (ECM) used in TSPA-1995 "behaved very sensitively" to the choice of "satiated matrix saturation" value. Unfortunately, the choice of 0.95 as a lower limit is not supported by laboratory or field information. Likewise, no mathematical basis is offered to support the limit. No information is presented in TSPA-1995 or in Xiang et al. (1995) to justify this important bounding value.

Available data from YM and from analogous systems suggest a limit less than 0.95 would be more appropriate. Fractures at YM are commonly coated with quartz, calcite, zeolites, and various clays and oxides (e.g., Carlos, 1987; Carlos et al., 1993) that may allow fracture flow to commence at matrix saturations well below 0.95. Field data from a system demonstrated to be similar in important regards to YM document that only a small fraction (0 to 5 percent) of the inventory of uranium transported along fractures has been partitioned into the tuff matrix (Pearcy et al., 1994; 1995). These field and laboratory data suggest that requiring matrix saturation of 0.95 for initiation of fracture flow is unrealistic and certainly not conservative.

Recommendations: The sensitivity of releases to lower limits for "satiated matrix saturation" should be investigated. Available field and laboratory data should be identified and used to develop a rational basis for a more realistic and more conservative bounding value.

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5 KEY TECHNICAL ISSUE: THERMAL EFFECTS ON FLOW

5.1 SCOPE OF REVIEW

The portions of TSPA-1995 relevant to the KTI concerning prediction of thermally driven redistribution of moisture through partially-saturated fractured porous media caused by emplacement of heat-generating high-level radioactive waste are identified in Table 5-1.

Table 5-1. Total System Performance Assessment 1995 scope of review for the Key Technical Issue: Thermal Effects on Flow

Section	Title
4.1	Introduction
4.2	Drift-Scale Thermal-Hydrology
4.3	Repository-Edge Thermohydrologic Calculations
5.3.3	Exposure Parameter Transformation
5.7.10	Alternative Thermal-Hydrologic Model
7.5	Transport of Gaseous-Phase Radionuclides

5.2 AREA OF CONCERN: CALCULATION OF TEMPERATURE AND RELATIVE HUMIDITY

5.2.1 Description of the Total-System Performance Issue

A significant conclusion of Chapter 10.2.1 of TSPA-1995 (p. 10-3) is that the thermohydrologic environment of waste packages (WPs) strongly affects the initiation and rate of aqueous corrosion. The thermohydrologic calculations presented in TSPA-1995 neither reference nor build upon previous analyses conducted for TSPA-1993 (Wilson et al., 1994). In addition, the results presented in TSPA-1995 have different trends than those in TSPA-1993, especially the evolution of the WP temperature prior to and after emplacement of the backfill. In TSPA-1993, the maximum WP temperature is obtained after backfilling and when it increases by about 330 °C (p. 10-26 of Wilson et. al., 1994). In TSPA-1995, the maximum WP temperature is obtained prior to backfilling, and the temperature increase is less than 20 °C (p. 4-24 of TSPA-1995). Another important difference is that a 2D model was used in TSPA-1995 where a 3D model was used in TSPA-1993. The 2D model is believed to average the WP heat source over a larger volume, hence tending to underpredict temperatures. Because the thermohydrologic environment of the WP affects many near-field processes important to TSPA, independent calculations were initiated to (i) reproduce the TSPA-1995 results using the same data and dimensions, and (ii) evaluate the differences introduced by using a 2D instead of a 3D model.

5.2.2 Description of the Department of Energy Approach and/or Position

In TSPA-1995 the FEHM coupled thermohydrologic code (Zyvoloski et al., 1995) is used to predict the evolving hydrothermal field near WPs. In TSPA-1993, similar calculations were performed using the COYOTE (Gartling, 1982) code. The similarities and differences in the calculations are compared in Table 5-2. Probably the most significant difference is that TSPA-1993 included a full 3D model of the WP residing in a drift while the TSPA-1995 uses a simpler 2D model. The TSPA-1993 results show a significant increase in WP temperature after backfill is emplaced (ΔT of about 330 °C increase from 190 to 520 °C), and the TSPA-1995 shows negligible effect (ΔT of about 15 °C increase from 150 to 165 °C). Some of the differences are explained by variations in (i) diameter of drift, (ii) conductivity of backfill, (iii) areal mass loading, and (iv) time of backfill. However, these differences do not fully explain the reported results.

5.2.3 Description of the Nuclear Regulatory Commission Approach and/or Position

Independent calculations have been performed by CNWRA in an attempt to reproduce the results in TSPA-1995 and to evaluate the impact of using a 2D model. The calculations have been performed for both the 25 MTU/acre and 83 MTU/acre Areal Mass Loading (AMLs). The calculations have been performed using the ABAQUS (1995) and MULTIFLO (Seth and Lichtner, 1996) codes. MULTIFLO simulates coupled heat and mass transfer in a porous medium which are the same processes included in FEHM which was used in TSPA-1995. ABAQUS simulates transient conduction heat transfer which is considered the dominant mode of heat transfer for low AMLs. Both codes are expected to yield comparable predictions for low infiltration rates. Thermal-geologic parameters are the same as those used in TSPA-1995 which are essentially the same as those used in TSPA-1993. A small portion of the computational mesh near the WP is shown in Figure 5-1 for the 2D mesh. Because the MULTIFLO code uses a rectangular grid, the WP and drift size are based on equivalent cross-sectional areas. The vapor pressure ratio is calculated using the same approach as Eq. 4.2-1 on Page 4-6 of TSPA-1995. The vapor pressure is the same as the relative humidity for below boiling conditions (below 97 °C) and is a measure of the tendency for liquid to exist on the surface. Within the emplacement drift, the absolute humidity is assumed to be uniform due to the relative ease with which vapor can flow within the drift. The actual vapor pressure at the WP surface is then dictated by the vapor pressure at the drift wall.

In Figure 5-2, TSPA-1995 results and CNWRA independent calculations are compared for the 25 and 83 MTU/acre cases. For the 2D, 25 MTU/acre results, the temperatures and vapor pressure ratio are in general agreement at long times. For the first few hundred years, the TSPA-1995 results show a higher WP temperature and resulting lower vapor pressure ratio. In general, the TSPA-1995 results show higher WP temperatures prior to backfilling. After reviewing the description in TSPA-1995, it is believed that this trend is due to underestimating the rate of radiative heat transfer from the WP to the drift wall prior to 100 yr. However, this could not be confirmed due to sparse documentation of the details in TSPA-1995. The report states that a radiative transfer model was employed but does not discuss how view factors were calculated nor does it discuss emissivity values for the package or drift wall.

For the 2D, 83 MTU/acre case, the temperature and vapor pressure ratio results are in better agreement. Again, the TSPA-1995 results show higher temperatures prior to backfill but essentially the same as the MULTIFLO code out to 10,000 yr. A curious anomoly in the TSPA-1995 results is that there is essentially no change in vapor pressure ratio due to backfilling the drift at 100 yr. As the WP temperature increases at backfilling, the vapor pressure ratio is expected to decrease but this trend is not evident in the TSPA-1995 simulation results.

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Table 5-2. Comparison of TSPA-1993 and TSPA-1995 thermohydrologic calculations

INPUT	TSPA-1993 (Wilson et al, 1994)	TSPA-1995 (TRW, 1995)
Code Used	COYOTE (Gartling, 1982) Conduction with adjusted specific heats to simulate boiling	FEHM (Zyvoloski et al., 1995) Multiphase, non-isothermal flow using finite element method
Geometry	3D waste package scale 7.62 m diameter drift	2D waste-package scale 5.0 m diameter drift
Thermal Loading	114 KW/acre (~125 MTU/acre) 11.88 m waste package spacing 25.4 m drift spacing	83 MTU/acre (~80 kW2/acre): 19 m waste package spacing 22 m drift spacing 25 MTU/acre (~24 kW/acre): 32 m waste package spacing 45 m drift spacing
Spent Fuel	26 yr from reactor 37.3 GWd/MTU average burnup (est. 9.3 MTU/cask)	23 yr from reactor 38.5 GWd/MTU average burnup (est. 8.8 MTU/pkg)
Host Rock Properties	Same as in TSPA-1995	Same as in TSPA-1993
Time of Backfill	75 yr	100 yr
Effective Conductivity of Backfill	0.2 W/(m-C)	0.6 W/(m-C)
Maximum Waste Package Temperature	520 °C at 75 yr	170 °C at ~15 yr for 83 MTU/acre 160 °C at ~10 yr for 25 MTU/acre
Waste Package Temperature Increase Promptly After Backfill Emplaced	330 °C	~15 °C both 25 and 83 MTU/acre
Relative Humidity Promptly After Backfill	not calculated	30% for 83 MTU/acre 50% for 25 MTU/acre

A 3D model is shown in Figure 5-3 and is used to predict WP temperature. The 3D model is motivated because the 2D model averages the heat source along the drift and this typically results in underpredictions of the WP temperature. The magnitude of the underprediction is uncertain, hence these calculations have been pursued. In Figure 5-4, the WP temperatures are compared for the 2D and 3D models using only the ABAQUS code. The 3D model more accurately captures the geometry and thermal evolution of the problem. After backfill, the near-field heat transfer around a WP is truly 3D. The results show that the 3D model predicts higher temperatures throughout the time of interest. Promptly after backfilling, the temperature difference is most distinct. For both the 25 and 83 MTU/acre cases, the WP temperature is about 80 °C higher for the 3D case promptly after backfill.

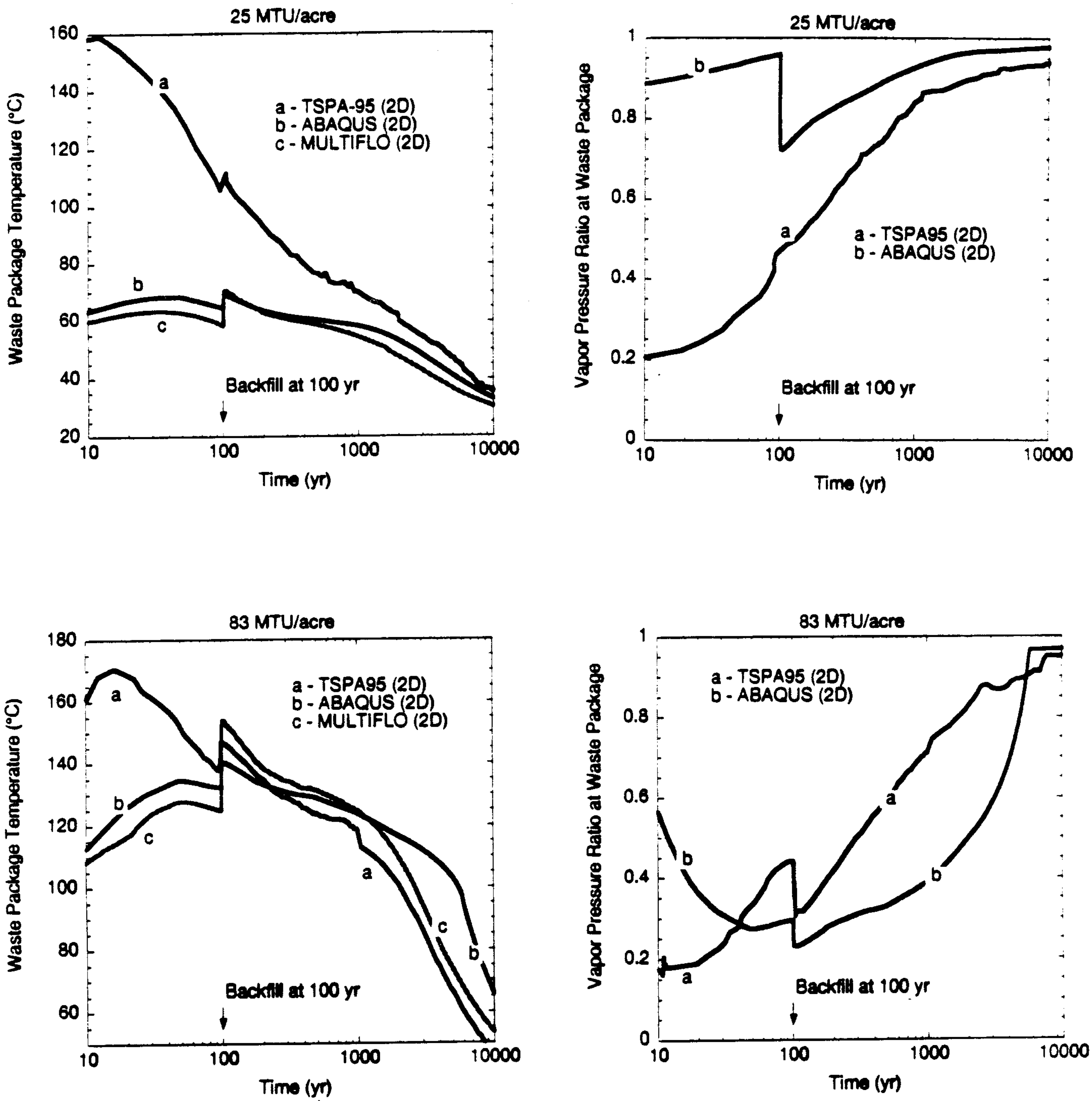

Figure 5-2. Results from two-dimensional model

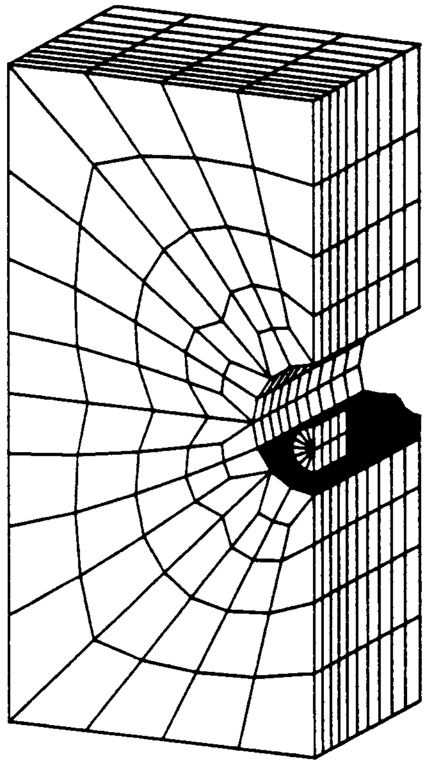

Figure 5-3. Three-dimensional model

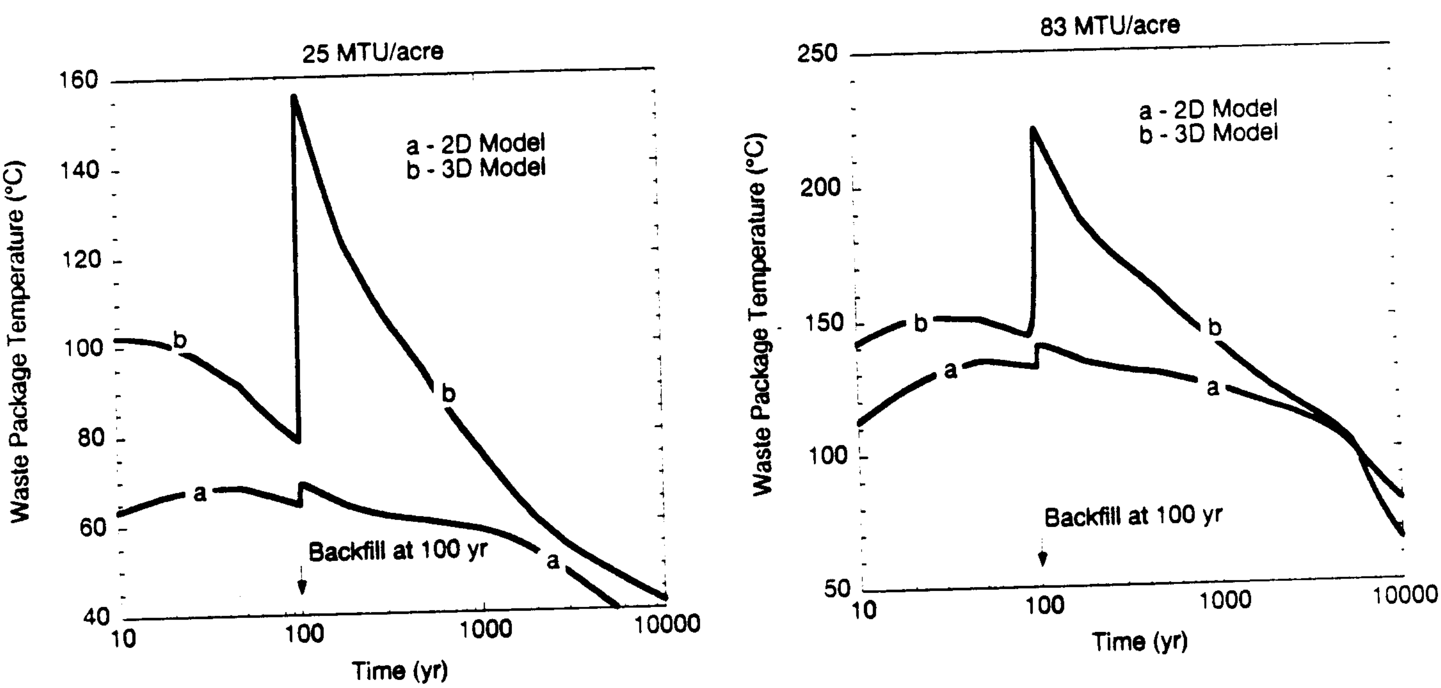

Figure 5-4. Comparison of two- and three-dimensional model results

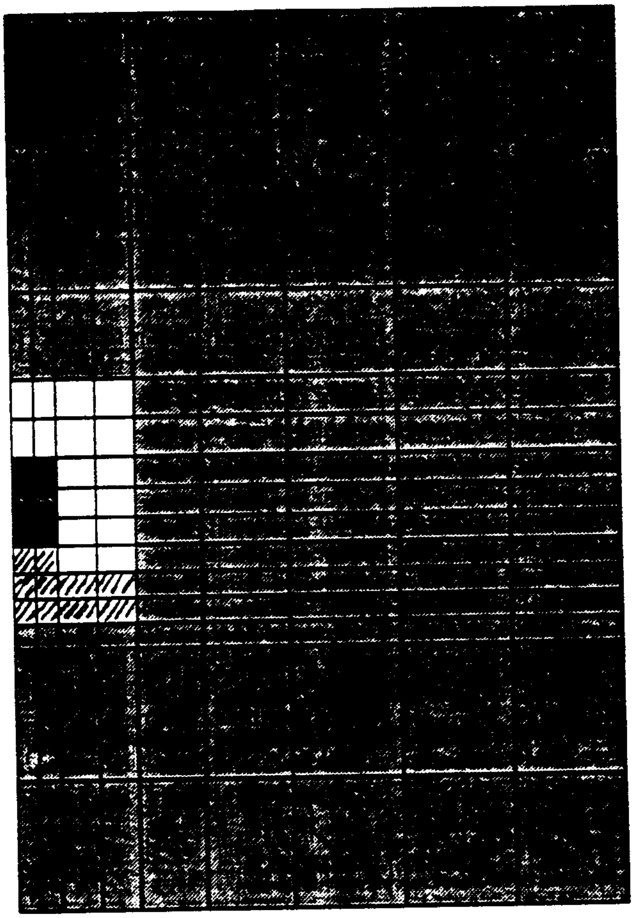

Figure 5-1. Two-dimensional model

5.2.4 Description of Likely Effects on Performance

Independent calculations conducted at the CNWRA were not able to reproduce some of the thermohydrologic results in TSPA-1995. In general, TSPA-1995 has higher WP temperatures before backfilling, and this is believed to be due to the radiative heat transfer model employed. However, the documentation of the model in TSPA-1995 is inadequate to fully explain the difference. The report does not discuss how view factors were calculated nor the emissivity values of the package and drift wall surfaces. In addition, the TSPA-1995 results do not have a significant temperature increase at the time of backfilling. As noted in TSPA-1995, different modeling assumptions can lead to significant differences in results. Assumptions about heat transfer mechanisms prior to backfilling are expected to be the cause of some differences.

The geometrical detail used to describe and simulate the near-field is another source of difference in predictions. The 2D model, such as employed in TSPA-1995, averages the heat source over the entire waste package spacing length. This tends to produce lower WP temperatures than a 3D model. The overall effect of lower temperatures may be conservative in the TSPA, but the discussion in TSPA-1995 does not claim to be bounding or conservative. It is reported as an unbiased estimate of anticipated conditions.

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Because the WP thermohydrologic environment is important to release and transport of radionuclides in the near-field, future TSPAs are encouraged to examine two areas of the calculations: (i) the heat transfer models in the drift prior to backfilling, and (ii) use of 2D versus 3D models.

5.3 GENERAL COMMENTS—THERMOHYDROLOGY

Statement of Concern: Three sets of analyses in TSPA-1995, Chapter 4 relate to thermohydrology: (i) a primary set of drift-scale analyses, (ii) an alternative drift-scale model (Buscheck et al., 1995), and (iii) a set of repository-edge calculations. All analyses were predicated on an equivalent continuum model (ECM) (Pruess et al., 1985) in which hydraulic equilibrium between fractures and the matrix is assumed. Justification for invoking an ECM was cited as: (i) a paucity of data on geometric/hydraulic characteristics of fractures at YM, and (ii) the computational complexity associated with modeling hydrothermal behavior in a discrete fracture network. ECM models have not been shown to be representative of groundwater flow through heterogeneous media. Consequently, the Chapter 4 interpretations of moisture redistribution at a HLW canister predicated on an ECM cannot be demonstrated as representative of the proposed repository at YM.

Basis of Concern: The assumption of hydraulic equilibrium between fractures and the matrix inherent in the ECM formulation precludes episodic fracture flow back to WPs. This or other fluid transport mechanisms not included in the ECM formulation could result in significantly different water contents or fluxes in the WP environment than those suggested by the thermohydrological analyses. The presence of water, either as bulk liquid water or as a thin film on the canister surface, can enhance the onset and rate of corrosion of the WP. Water transport models are required which accurately incorporate the mechanisms which dictate the saturation, flux of water through either the matrix or fractures and the time at which water re-enters the near-field environment of the WP subsequent to the onset of heating. The omission of a mechanism such as episodic fracture flow from an ECM suggests that results drawn from the analyses are not conservative (Pruess and Tsang, 1993; 1994; and Wittwer et al., 1995).

Recommendations: The lack of conservatism in the thermohydrologic modeling can be assessed, at least in part, by comparing the ECM formulation results with results derived from alternative conceptual models. For example, one possible alternative conceptual model could be formulated from dual-porosity and/or dual-permeability representations. Additional alternative conceptualizations could be taken from a discrete fracture flow model or from an ECM model in which the hydraulic equilibrium requirement is relaxed. These flow models could be used to investigate the relative importance of episodic fracture flow and provide evidence to test whether the ECM formulation adequately incorporates the important fluid transport mechanisms expected at the proposed repository.

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6 KEY TECHNICAL ISSUE: CONTAINER LIFE AND SOURCE TERM

6.1 SCOPE OF REVIEW

The portions of TSPA-1995 relevant to the KTI concerning the prediction of container life and radionuclide release over long periods in a deep geologic repository environment are identified in Table 6-1.

Table 6-1. Total System Performance Assessment 1995 scope of review for the Key Technical Issue: Container Life and Source Term

Section	Title
3.5	Waste Package Design
3.7	Radionuclide Inventory
5.1	Introduction
5.2	Corrosion Modes
5.3	Humid Air Corrosion Models for Corrosion
5.4	Aqueous Corrosion Models for Corrosion Allowance Materials
5.5	Corrosion Modeling of Corrosion Resistant Materials
5.6	Cladding Degradation
5.7	Waste Package Degradation History
5.8	Summary and Recommendations
6.1	Introduction
6.2	Waste Form Alteration Modeling
6.5	Radioactive Release Modeling

6.2 AREA OF CONCERN: WASTE PACKAGE FAILURE MODES

6.2.1 Description of the Total-System Performance Issue

The current conceptual design of the WP for spent fuel and vitrified defense high-level waste (DHLW) [Department of Energy, (1994)] was evaluated in TSPA-1995 using a stochastic WP performance model. This most recent design is a significant departure from the single-wall container concept evaluated in TSPA-1993 (Wilson et al., 1994). The design consists of an outer disposal overpack made of a corrosion-allowance material (carbon steel) and an inner container made of a corrosion-resistant alloy (alloy 825). An additional containment barrier of a moderately corrosion resistant material such as alloy

400 is included in the low thermal-load repository design (Department of Energy, 1994). However, this additional containment barrier was not considered in TSPA-1995 based on the argument that models for predicting the performance of this type of material are not currently available. Also, the multipurpose canister (MPC) made of type 316L stainless steel and the pour canister for DHLW are not included in TSPA-1995, since no credit is assigned by the DOE to these canisters as containment barriers.

Although several corrosion modes, including crevice corrosion, stress corrosion cracking, microbially influenced corrosion and galvanic corrosion, are briefly mentioned in an introductory discussion (TSPA-1995, pp. 5-2 and 5-3) as potential failure modes for the WP, the performance calculations in TSPA-1995 include only general corrosion and pitting corrosion. It is stated, however, that the carbon steel outer barrier will provide some degree of cathodic protection to the alloy 825 inner container through galvanic coupling.

The WP performance calculations presented in Chapter 5 of TSPA-1995 are considered to be nonconservative because:

- Relevant failure modes, such as crevice corrosion, stress corrosion cracking, microbially influenced corrosion and thermal embrittlement of steel, are not included in the analysis.

- The chemistry of the environment contacting the WP does not correspond to bounding environments described in the DOE long-term testing program (Lawrence Livermore National Laboratory, 1995a)

6.2.2 Description of the Department of Energy Approach and/or Position

In general terms, the approach adopted in TSPA-1995 regarding WP degradation is consistent with the hypothesis on waste containment presented in the document on the DOE Waste Containment and Isolation Strategy for the Yucca Mountain Site (TRW Environmental Safety Systems, 1995). In particular, the WP environment in both documents is considered to be hot air with the presence of water vapor.

In the TSPA-1995 report, humid-air corrosion is considered to be corrosion which takes place under a thin film of water that forms on the container surface above a critical relative humidity range uniformly distributed between 65 and 75 percent. Aqueous corrosion refers to corrosion of metal in contact with bulk water, assumed to occur at relative humidities greater than a threshold value uniformly distributed between 85 and 95 percent.

The conceptual model for humid-air corrosion of the outer steel container is based on assuming an exponential dependence of the corrosion rate with the relative humidity (RH), the inverse of absolute temperature (T) and the concentration of SO_2 in the environment ($[SO_2]$), in addition to a power dependence of the general corrosion depth (D_g) with time (t), which leads to the following expression

$$\ln D_g = a_0 + a_1 \ln t + a_2/RH + a_3/T + a_4[SO_2] \tag{6-1}$$

The parameters a_i in Eq. (6-1) were obtained from linear regression of 166 data points acquired from atmospheric corrosion exposures in different locations extended up to a total time of 16 yr, using a specific equation to account for the time fraction during which the relative humidity was greater than

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70 percent. Pitting corrosion was treated by using a pitting factor in order to obtain pit depth from the general corrosion penetration in humid air.

An expression similar to Eq. (6-1) was used for general corrosion of the outer steel container under aqueous conditions

$$\ln D_g = b_0 + b_1 \ln t + b_2/T + b_3 T^2 \tag{6-2}$$

The parameters b_i in Eq. (6-2) were obtained from long-term (up to 16 yr) corrosion data acquired in polluted river water and tropical lake water combined with short-term (100 days) corrosion data for the temperature effect. As in the case of the humid-air environment, pitting corrosion was evaluated from general corrosion calculations by assuming a pitting factor.

Humid-air corrosion was assumed to be negligible for the inner corrosion-resistant container, as well as for the case of general corrosion in the aqueous environment. For pitting corrosion in an aqueous environment the median pit growth rate was expressed as

$$\ln R_p = A - 0.5 \ln t - B/T \tag{6-3}$$

where R_p is the pit growth rate in mm/yr and A and B are constants.

By using temperature and humidity profiles at the WP surface obtained from thermohydrologic modeling and Eq. (6-1) through (6-3), stochastic simulations of WP degradation were performed by adopting a set of additional assumptions which will be the subject of detailed examination in a further review of TSPA-1995.

6.2.3 Description of Nuclear Regulatory Commission Approach and/or Position

The NRC considers that the definition of the WP environment adopted by the DOE and the failure modes arising from the interaction of this type of environment with the WPs may not lead to a conservative assessment of performance because this assessment is based on a simplified consideration of atmospheric corrosion. Among other aspects, the relative humidity criterion, based only on ambient temperature observations without considering the hygroscopic nature of corrosion products or other forms of capillary condensation (Leygraf, 1995; Fyfe, 1994), may be nonconservative.

Evolution of the near-field environment with time (Sridhar et al., 1995) is not properly addressed in the TSPA-1995 analysis of WP performance. The possibility of fracture flow and concentration of anionic species in the groundwater as a consequence of thermohydrologic effects (Walton, 1993) and chemical interactions with minerals (Abraham et al., 1986) is not included in the analysis and therefore, contact of liquid water or concentrated saline solutions with the WP surface are not anticipated at shorter times than those predicted by the relative humidity criterion. Consideration of these factors, in particular concentration of groundwater by alternative wetting and drying processes, may alter significantly the results of the performance evaluation conducted in TSPA-1995 and their effects must be quantified.

Use of Eq. (6-1) for evaluating corrosion of the outer steel barrier may lead to nonconservative estimates of the extent of corrosion. Equation (6-1) does not contain terms for the effect of aggressive species, with the exception of SO_2, which is not expected to prevail in the repository environment. The inclusion of atmospheric environments containing chloride, which is one of the most detrimental anionic species, was omitted from the atmospheric corrosion database used to obtain the parameters a_i. This omission was justified stating that marine environments are much more corrosive than the near-field environment considered in TSPA-1995. The aqueous corrosion model described by Eq. (6-2) does not include the important effects of pH, redox species (or corrosion potential), and other environmental factors, such as chloride concentration, that may be relevant to the corrosion of the outer steel overpack.

In general terms, long-term predictions using simple logarithmic power laws may underestimate long-term corrosion rates, particularly when the database covers a very limited time span (16 yr) compared to the extrapolation time (thousands of years). Power linear models and composite models have been shown to better fit long-term corrosion data according to McCuen and Albrecht (1994), but other extrapolation approaches should be considered.

Using linear regression fits to determine the parameters needed in the models introduces uncertainty in both intercept and slope. Statistically, the uncertainty is at a minimum at the mean of the data (Hays, 1973) and increases above and below the mean. However, the curve fits to the data for the corrosion models exhibited constant uncertainty, indicating that the uncertainty involved in applying these models for periods up to 10^5 yr is underestimated.

The use of a pitting factor, with a normal distribution around a mean of 4 and a standard deviation of 1 for both humid-air and aqueous corrosion stochastic calculations, appears to be questionable. Larger variations can be expected. McCright and Weiss (1985) reported a pitting factor greater than 9 for 1020 steel in J-13 water at 100 °C after 5,000 hr exposure, whereas data reviewed by Vinson et al. (1995) revealed penetrations at pits of at least 10 times the general corrosion values. Although the cumulative distribution functions for pit depth reported in TSPA-1995 seem to exhibit a consistent and reasonable trends (as a function of environmental variables such as temperature, relative humidity, exposure time, etc.), the quantitative predictions may not be sufficiently accurate.

The lack of dependence of pitting corrosion on chloride concentration and corrosion potential, for a corrosion-resistant alloy such as reflected in Eq. (6-3) for alloy 825, is contrary to the findings reported in a large body of literature (Szklarska-Smialowska, 1986). As a consequence, the calculations may be nonconservative for a wide range of conditions encompassing relatively large chloride concentrations and high corrosion potentials. Relatively high corrosion potentials may arise not only from the presence of air but also from a combination of factors, including oxidizing species generated by radiolysis if localized breaching of the thick outer container occurs prematurely and groundwater contacts the inner container. The concept of cathodic protection as a result of galvanic coupling is valuable, but requires a more accurate evaluation. The lack of an electrolyte as a conducting medium, which is accepted as a plus for the extended integrity of the outer container, may in turn limit the throwing power (or protection capability) of the cathodic current to closely contacting areas.

Although dry oxidation is not considered an issue in TSPA-1995, the potential for grain-boundary oxidation at low temperatures (below 350 °C), facilitated by grain boundary diffusion of oxygen, needs to be evaluated. This is a well established phenomenon a higher temperatures (Newcomb and Stobbs, 1991), but its potential incidence at repository temperatures should be considered. Even more important as a potential failure mode is the thermal embrittlement of the outer steel overpack, particularly in welded areas. Thermal (or temper embrittlement) of low-alloy steels used for pressure vessels is a well established phenomenon which is related to phosphorus segregation to grain boundaries (or that of other equivalent impurities such as arsenic, tin, and antimony) and a concomitant decrease of fracture toughness, as revealed by the drop of the impact energy measured in Charpy tests. The existence of a similar effect on C-Mn steels after extended exposure times to temperatures around 200 to 300 °C may have a significant effect on performance that requires consideration in TSPA-1995. Although calculations are needed to establish a conservative criterion, stresses arising from seismic events or present as residual stresses, may be sufficient to induce fracture if the material is embrittled.

Variability in the corrosion models is arbitrarily partitioned between spatial variability in performance and uncertainty in model parameters. Spatial variability is likely in the repository, resulting, as an example, from temperature variations related to variable thermal loads in WPs and/or position of the WPs in the repository. The arbitrary partition between spatial variability in performance and uncertainty in model parameters is a nonconservative approach, which distributes failures and releases over time, thereby reducing peak release and dose. The delayed onset of dripping may cause pulsed release of radionuclides beyond the steady-state release.

6.2.4 Description of the Likely Effects on Performance

Most of the limitations of the corrosion models adopted by the DOE, as discussed above, may lead to a nonconservative assessment of performance. The most important factor appears to be related to the selection of the conceptual models and the lack of consideration of several relevant failure modes. With the exception of thermal embrittlement, however, the lack of consideration of other failure modes, such as crevice corrosion, stress corrosion cracking, and microbially influenced corrosion, in the simulations of WP degradation is acknowledged in the current iteration presented in TSPA-1995.

An additional factor that may influence the assessment of performance is the restricted database selected for the determination of the relevant equations and the parameters involved, combined with limitations of the functional dependence used in the various models. The selection of an inadequate functional relationship may lead to significant differences with respect to more accurate expressions when data obtained over a period of few years is extrapolated to predict the behavior after thousand of years. No indication of approaches to deal with this level of uncertainty is presented in TSPA-1995. Underestimating uncertainty concerning corrosion models results in a lower probability of early container failure realizations. Earlier release of radionuclides increases the cumulative releases to the accessible environment.

Arbitrary partitioning of uncertainty into spatial variability spreads WP failures and EBS release rate over longer time intervals thereby lowering peak EBS releases and maximum dose. Spatial variability should be demonstrated using mechanistic arguments.

6.3 GENERAL COMMENTS—WASTE PACKAGE BARRIERS

6.3.1 General Comment—Cladding Degradation Modes

Statement of Concern: The dominant failure modes of Zircaloy fuel cladding considered in TSPA-1995 are creep rupture and cladding splitting. The equations for time to failure of the cladding by creep (Santanam et al., 1992) and the rate of cladding "split" growth (Einziger, 1994) are based on an empirical fit to the data. Although the cladding "split" growth rate is based on properties of irradiated cladding, the data used to develop the empirical relations for creep strain appears to be relevant to unirradiated cladding and, therefore, may not provide reasonable estimates for spent fuel cladding.

Basis of Concern: The mechanical properties that determine the creep rupture life of cladding can be modified due to irradiation of the fuel in a power reactor. Irradiation-induced hardening has a deleterious influence on the creep strength of cladding and can therefore result in a lower time-to-failure for the cladding.

Recommendations: The creep failure of the cladding should be based on properties of irradiated Zircaloy fuel cladding.

6.3.2 General Comment—Waste Form Alteration and Radionuclide Release

Statement of Concern: The TSPA-1995 assessment of the source term may not be conservative. Five areas of uncertainties can be identified.

(i) Effects of dry oxidation on the surface area and consequent dissolution of spent fuel is inadequately recognized.

(ii) Colloidal release is not included in performance calculations.

(iii) Enhanced release of fission products and gaseous release from fuel are neglected.

(iv) Although it was concluded that the EBS peak release rate performance measure depends strongly on rate of spent fuel dissolution, treatment of the rate of spent fuel dissolution is ambiguous in many regards.

(v) Equations (TSPA-1995 Eqs. 6.2-2 and 6.2-3) developed for the dissolution of glass waste forms as a function of pH and temperature of the leachate do not account for the concentrations of ionic species that are known to enhance the dissolution rate of glass.

Basis for Concern:

(i) In TSPA-1995 dry oxidation of spent fuel for [O/U] ratios below 2.4 is assumed not to increase surface area significantly for subsequent matrix dissolution, and matrix dissolution is presumed to be proportional to the exposed surface area. Upon dry oxidation for [O/U] ratios above 2.4, the surface area is expected to increase by a factor of 100 as a result of the exposure of individual grains to leachates. Transgranular fractures are not considered in the TSPA-1995 analysis. However, recent DOE experimental results (Lawrence Livermore National Laboratory, 1995b) indicate that individual grains may be exposed to leachates when preoxidized spent fuel with [O/U] ratios below 2.4 is immersed in J-13 well water. The exposure of individual grains implies that dry oxidation increases surface area. Also, when fuel fragments are oxidized to [O/U] ratios above 2.4, transgranular fracturing can take place (Gray and Wilson, 1995), which may further increase surface area above the factor proposed in TSPA-1995.

(ii) Colloidal release of actinides is discussed in TSPA-1995, and the report concludes that actinide release would be increased by a factor 3 by the colloid contribution. However,

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there is no explicit treatment of the role of colloids in the release or dose computations of the TSPA. Dissolution tests with dripping ground water indicate large amounts of Pu and Am releases (Finn et al., 1994). It is possible that these releases are associated with colloids, and colloids may be transported along fracture paths of host rocks without significant retardation. Even if colloids grow and settle out of solution because of gravitational forces, there is a possibility of colloidal transport by convective flow of groundwater, especially through vertical host-rock fractures. Neglecting the contribution of colloids to the source term may be nonconservative.

(iii) It is assumed in TSPA-1995 that fission products and activated radionuclides (i.e., C-14) are released in proportion to the matrix dissolution rate. Also, solid state diffusion is not considered. However, fission products and C-14 can be released by solid state diffusion. This is a more likely scenario when spent fuel is subject to a prior dry oxidation. For instance, Xe (which is similar in size to I-129) diffusivity increases by many orders of magnitude at around 1000 °C as the matrix is oxidized (a summary in Nicoll et al., 1995). The discrepancy between diffusivities in unoxidized and oxidized spent fuel would be more significant as temperatures decrease. C-14 may diffuse to the surface even without prior dry oxidation (Ahn, 1994). The release by solid matrix diffusion would lead to early release of fission products and C-14. For instance, if C-14 diffusion kinetics follow oxygen diffusion kinetics, all matrix C-14 may be released from the fuel above 73.5 °C within 10,000 yr (Ahn, 1994). Another example is I-129 release. If diffusivity is greater than 3×10^{-18} cm^2/sec, all matrix I-129 would be released from the fuel within 10,000 yr (Ahn, 1995a). This fast diffusion-induced release may be likely if spent fuel is subject to dry oxidation (e.g., Nicoll et al., 1995). Dry oxidation can result in amorphization and fracture (Lawrence Livermore National Laboratory, 1995b; Gray and Wilson, 1995), both of which increase diffusion rates. This general behavior would apply to other radionuclides such as Cl-36, Tc-99 or Cs-135.

(iv) An empirical equation in TSPA-1995 (6.2-1) is provided which is a regression of data for the rate of dissolution of spent fuel as a function of temperature, pH, and total carbonate concentration. Presumably a subset of the data and the regression curves are provided in TSPA-1995 Figures 6.2-1 and 6.2-2. However, the pH value used to generate the curves is not indicated in the report. The range of the ±2 standard deviations for a given temperature and pH is about 1 order of magnitude. There is apparently a great deal of scatter in the data relative to the overall range of regressed variation, which is also about an order of magnitude. It appears that the same curves are plotted in Figure 6.2-4 in linear coordinates and with different units. However, a comparison of the two sets of curves reveals that they are different. For example, for total carbonate equal to 0.002 M at 100 °C the value from Figure 6.2-1 is 21 $mg/m^2/day$ which equals 7.67 $g/m^2/yr$, but the value for the same conditions in Figure 6.2-4 is 13 $g/m^2/yr$. Similarly, for total carbonate equal to 0.02 M and 100 °C, the respective values corresponding to curves in Figures 6.2-2 and 6.2-4 are 14.6 $g/m^2/yr$ and 25 $g/m^2/yr$. The ratios are the same, so it may be a good guess that the figures were generated for different unstated pH values.

It is apparently unstated in TSPA-1995 Chapters 6 or 8 how the dissolution rate regression (Eq. 6.2-1) was used to generate a distribution function for rates of spent fuel dissolution. It is unclear how temperature, carbonate, and pH were selected. It is noted with respect to solubilities that "the near-field pH evolution is uncertain to the extent that adequate constraints do not exist for making a pH choice other than a random selection from a distribution," so a unique value of pH 7 was used in the "alternative solubility models."

Nevertheless, the significance of the functional relation of the dissolution rate to temperature, pH and carbonate is questionable considering that the range of variation in rate for the regressed curves nearly corresponds to the range of variability in the data for a given temperature and pH, and considering the formidable uncertainties in surface area, which may extend orders of magnitude.

(v) The effect of the enrichment of groundwater with WP corrosion products on the dissolution rate of glass waste forms is not considered in TSPA-1995. The empirical equations developed for the dissolution of glass are based only on pH and temperature and do not account for the concentration of ionic species which are likely to be present in the groundwater and are known to accelerate the dissolution rate of glass (McVay and Buckwalter, 1983). One such species is $Fe(3+)$, which is expected to be present in groundwater as a result of corrosion of the WP components. It is also unclear whether the empirical glass dissolution rate equations provided in TSPA-1995 are bounding rate equations for all compositions of borosilicate glass anticipated for disposal. The current DOE designs call for an overpack of carbon steel for the WP. Continuous release of Fe ions from the overpack will prevent the groundwater from reaching the solubility limit of silica, thereby preventing the asymptotic leveling of the glass dissolution rate observed in closed systems in the absence of Fe ions in the leachate. Therefore, the long-term dissolution rate of glass waste forms could be much higher than that estimated without the presence of corrosion products in the groundwater.

Recommendations:

(a) Current Pacific Northwest Laboratories (PNL) (Gray and Wilson, 1995) experimental results need to be incorporated in PA.

(b) Future Argonne National Laboratory experimental results need to be interpreted, modeled and incorporated in PA. (For sample models, see Ahn, 1995b; Manaktala et al., 1995)

(c) Future PNL experimental results and some data from reactor operation may need to be used in PA.

(d) Clarify parameters used to generate dissolution rate figures, and explain how parameters were generated for use in Equation 6.2-1 to calculate spent fuel dissolution rates.

(e) The glass dissolution rate equations should be modified to incorporate the influence of ionic species that are known to accelerate the dissolution rate of glass.

6.3.3 General Comment—Limits of Capillary Barriers

Statement of Concern: TSPA-1995 assumes that a capillary barrier can ensure diffusion only release from WPs. Capillary barriers are potentially a very significant additional barrier for the YM proposed repository and should be considered. However, capillary barrier performance is very sensitive to the (i) unsaturated flow properties of the overlying conductive layer, (ii) pore size distribution of the lower capillary break layer, (iii) the infiltration rate, and (iv) spatial and temporal distribution of infiltrating water.

Basis of Concern: Proper functioning of a capillary barrier requires that unsaturated flow in the upper conductive layer wick moisture under tension around the WP. If saturation is approached anywhere along the bottom of the conductive layer, the capillary barrier fails, leading to dripping on the waste container and associated advective releases. The limitation of unsaturated flow places an upper bound on the capacity of a capillary barrier to divert infiltrating water. Equations for the diversion capacity of a capillary barrier or the simple case of constant infiltration have been developed by Ross (1990) and are applied in Walton and Seitz (1992).

The case of localized flow (e.g., caused by fracture dripping) and transient dripping events is computationally more complex but amenable to numerical simulation. The more complex problem is addressing changes in the properties of the porous medium around the WP over time as a result of heating. The strong matric suction obtained in tuff rock tends to focus evaporation at the edge of the drifts. Infiltration episodes along fractures will also periodically wet the upper conductive layer and then be evaporated at the higher temperatures (the granular materials required for a capillary barrier have lower thermal conductivity than the surrounding tuff rock leading to higher waste package temperatures). When the water evaporates, minerals precipitate, thereby changing the pore size distribution of the conductive layer. Anticipated water reflux and fracture drip rates are sufficiently high to lead to significant changes in material properties over time. Formation of layers of precipitated calcite and/or silica in the conductive layer at the point of evaporation may lead to failure of the capillary barrier.

Failure of a capillary barrier causes the WP involved to be subject to advective release. Based upon TSPA-1995 (Figure 9.3-44, p. 9-83), capillary barriers can reduce the dose by up to a factor of 10,000 when compared to the nominal case.

Recommendation: Capillary barriers around the WP can lead to large improvements in WP performance and are potentially one of the most effective barriers available at an unsaturated site. At the same time, the performance characteristics of capillary barriers are sensitive to a variety of processes active at the YM proposed repository. Future PAs should consider the conditions under which capillary barriers can be sustained and the uncertainties related to their performance as a consequence of heating and coupled effects.

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7 KEY TECHNICAL ISSUE: STRUCTURAL DEFORMATION AND SEISMICITY

7.1 SCOPE OF REVIEW

The portions of TSPA-1995 relevant to the KTI concerning the development and use of tectonic models to assess future structural deformation and seismicity magnitudes are identified in Table 7-1.

Table 7-1. Total System Performance Assessment 1995 scope of review for the Key Technical Issue: Structural Deformation and Seismicity

Section	Title
2.7.3	Tectonic Effects

7.2 GENERAL COMMENTS—DISRUPTIVE EVENTS AND PROCESSES

7.2.1 General Comment—General Conclusions Not Supported by Citations

Statement of Concern: The conclusions in TSPA-1995 that probability-weighted releases associated with fault-slip and seismicity (p. 1-4) and that consequences of potential seismicity on total system performance are negligible (p. 2-12) are not justified by studies cited as supporting these conclusions. These events and processes are potentially important to WP, (i.e., WP failure resulting from structural failure) and total systems performance and should be incorporated in the calculation of a CCDF.

Basis of Concern:

(i) Auxiliary study of the effects of faulting and seismicity on total system performance (Gauthier et al., 1995) concludes that under certain conditions (e.g., fracture flow with no backfill) an order of magnitude increase in release was anticipated.

(ii) Gauthier et al. (1995) also concludes that additional data and further analyses are needed to adequately define the impact of seismic effects on the potential repository.

(iii) Previous total system performance studies (e.g., Nuclear Regulatory Commission, 1995 and Wilson et al., 1994) greatly oversimplify and do not accurately constrain faulting and seismicity in the YM region with the intention that such complexities would be considered in subsequent iterations. Conclusions about possible effects of faulting and seismicity on total system performance drawn from these earlier studies are not necessarily valid.

(iv) The available data support other interpretations of a conceptual framework for the effects of faulting and seismicity on total system performance that may lead to higher consequences than those postulated under the analyses used to justify not considering fault slip and seismicity.

Recommendations:

(i) Accurately portray conclusions from supporting studies in justifications about the significance of faulting and seismicity on total system performance.

(ii) Reserve judgement on effects of structural deformation and seismicity on total system performance until further iterations of TSPA and Probabilistic Seismic Hazard Analysis (PSHA) are carried out. These additional studies should be based on conceptualizations of faulting derived from viable tectonic models and data consistent with all available fault slip and seismicity data.

7.2.2 General Comment—Faulting and Seismicity

Statement of Concern: Faulting and seismicity were not directly considered in TSPA-1995. Their potential effects on TSPA were prematurely discounted on the basis of auxiliary PSHA analyses. Data on faulting and seismicity used in auxiliary studies support other interpretations that have greater consequences (i.e., early canister failures and creation of fast pathways).

Basis of Concern:

(i) Fault-slip estimates do not incorporate all available paleoseismic data.

- For example, fault-slip estimates for the Death Valley-Furnace Creek fault are given as a slip rate of 2–4 mm/yr and a recurrence interval of 1,000 to 4,000 yr (Table 1 of Wong et al., 1995). Yet, recent work by the USGS indicate slip rates of 4–7 mm/yr and possibly as high as 12 mm/yr with a recurrence interval of 500–1,000 yr (Reheis, 1994).

- Doubling the slip rate (from 4 to 8 mm/yr, for example) could increase either the number of earthquakes or the magnitude of the maximum earthquake by a factor of two or more.

(ii) Fault-slip estimates for the YMR (see e.g., Wong et al., 1995, Table 1) are lower than other existing estimates not used by the DOE.

- Other methods of estimating slip indicate significantly greater slip rates. For example, recent work at Bare Mountain (BM) (Ferrill et al., 1995) based on kinetic models of the partial annealing apatite fission tracks yield slip-rates up to ten times greater than those derived from trenching studies.

- Geodetic measurements near BM (Ferrill et al., 1995; Gilmore, 1992) indicate slip-rates up to one order of magnitude greater than maximum values from trenching studies. Such results imply that either the trenching-based paleoseismic estimates grossly underestimate past slip rates or that the current period is anomalous.

(iii) Fault-slip estimates from trenching studies in alluvium do not necessarily identify maxim slip-rates or most frequent recurrence intervals. (see e.g., Wong et al., 1995, Table 1).

- Estimates of fault activity are sensitive to location of the trenching site. Most normal faults show considerable differential displacement along the length of the fault (e.g., Dawers et al., 1993). Down-dip displacement along the Solitario Canyon Fault, for example, increases by 1 m over a horizontal distance of 10 km (Scott, 1990).

- Recent studies of the distribution of alluvial fans around BM (Ferrill et al., 1995, Ferrill et al., in press) show significant differential movement along the BM Fault, including evidence for Holocene slip at the southern end of the mountain in contrast to the location of the surface trench at the northern end of the mountain (Klinger and Anderson, 1994).

- Estimates of fault slip from surface trenching studies do not account for possible distributed slip, in which only a portion of the total slip is captured by the trenched fault.

(iv) Fault-slip estimates do not incorporate all components of fault-slip (see Wong et al., 1995 Table 1).

- Fault-slip is the amount of displacement along the fault parallel to the slip direction not the amount of vertical (throw) or horizontal (heave) offset commonly reported as fault-slip. Throw or heave rates were apparently not corrected for plunge of the slip vector in auxiliary PSHA study (Wong et al., 1995). Because throw or heave are only a component of the total slip, correction for the true slip vector will necessarily increase slip-rates.

(v) The Exploratory Studies Facility (ESF) PSHA study concluded that historic seismicity is greater than that predicted from the paleoseismic data (Quittmeyer et al., 1994). This mismatch suggests that one or both data sets are not representative of expected seismicity. Yet, both the historic and paleoseismic data are used in the PSHA; the historic record as an estimate of background seismicity (aerial source term) and the paleoseismic record for seismicity on known faults (fault source term).

(vi) Blind seismic sources that do not produce surface rupture are not captured by trenching studies and are not considered in assessment of the paleoseismicity data.

- In the TSPA and PSHA studies it is assumed that all faulting with magnitudes greater than M=6.0 to M=6.5 will produce surface rupture (Wong et al., 1995). This assumption is based on a vertical, square rupture plane and a 15 km thick brittle-elastic upper crust. Yet, recent earthquakes at Northridge (M=6.9) and Big Bear (M=6.7), California did not produce any recognizable surface offset.

(vii) Threshold magnitude used to define aerial source term is too large and results in an inappropriate underestimation of seismic risk. In addition, the assumption in Gauthier et al. (1995) that only M=6.0 to M=6.5 could cause fault displacement in the repository block is not justified.

- Smaller earthquakes (M=5.7-6.0) are capable of offsets on the order of 10^{-1} m (Wells and Coppersmith, 1994).

Recommendations:

(i) DOE analyses should be consistent with all relevant data and DOE should justify why it is not using some relevant data.

(ii) Methods of estimating fault slip other than fault-trenching studies should be included in fault slip estimates.

(iii) Alternative methodologies of fault slip need to be used to assess differential slip.

(iv) Correct all slip-rates for fault geometry and slip vector. Corrections should be accurately reported in summary tables of fault-slip parameters.

(v) Reassess paleoseismic estimates and reconcile differences between the two terms.

(vi) Account for the possibility of undetected slip and large magnitude ($M \leq 6.9$) earthquakes on blind faults in PA, TSPA, and PSHA studies.

(vii) Alternative models should be run using a lower magnitude background earthquake (e.g., $M=5.7$), which appears to be a more prudent value (Hofmann and Ibrahim, 1995). PSHA studies should be regenerated using these more prudent and conservative values. The consequences of these smaller offsets on known faults should also be incorporated in TSPA and PSHA calculations.

7.2.3 General Comment—Seismically Induced Water-Table Changes

Statement of Concern: The conclusion in TSPA-1995 that seismically induced changes in the level of the water-table would be insufficient to reach the potential repository is based on nonconservative estimates of fault slip and an inaccurate representation of fault geometries. Water-table rises that do not reach the repository horizon shorten the unsaturated zone travel path potentially degrading repository performance.

Basis of Concern:

(1) In the performance assessment studies of Gauthier et al. (1995) three types of faults were modeled: (i) a high-angle normal fault with a 60° dip, (ii) a detachment fault with a 5° dip and dip-slip displacement, and (iii) a right-lateral strike-slip fault with a 60° dip. Only the strike-slip fault showed a significant effect and only the consequence of direct water-table intersection in repository was considered significant.

- All strike-slip faults in YMR have dips significantly steeper than 60°.

- Strike-slip faults in other aspects of PSHA and PA studies are modeled with 70–90° dips.

- The possibility that tectonically induced long-term water-table rise could also affect transport to accessible environment was not considered.

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(ii) The simulated earthquake (M=6.5 with 1 m of displacement along a 30 km rupture length) is not conservative.

- In some tectonic settings (e.g., DePolo et al., 1991) similar to ones proposed for Crater Flat (Fridrich et al., 1994) large-magnitude (M>7.0) earthquakes rupture multiple and complex fault segments, which otherwise, based on their individual fault lengths, would not seem capable of supporting such large-magnitude events. The potential effects of these larger-magnitude earthquakes on water-table rise and fracture dilation need to be considered in future TSPA studies. Repetitive larger-magnitude earthquakes could potentially modify, more quickly, the preferential flow paths in rock mass surrounding the repository.

- Recent global positioning system data suggest that up to 20 m strain could accumulate in the YMR in the next 10,000 yr. This strain accumulation would be sufficient to produce up to seven earthquakes in the M=6.5 to M=7.5 magnitude range (Ferrill et al., 1995).

Recommendations:

(i) Seismic terms and geometries of faults used in total system performance studies need to be constrained by conceptual tectonic models in order to more accurately estimate the consequences of their effects on the saturated zone hydrology and resulting changes in the path length between the repository and the water table.

(ii) More conservative estimates of the number and magnitude of earthquakes need to be used in total system performance and auxiliary PSHA studies. The effects of larger and more frequent earthquakes will have both temporary and permanent effects on the saturated zone and the average path length between the repository and the saturated zone should be considered in future studies.

7.2.4 General Comment—Tectonic Effects on Flow

Statement of Concern: Underestimation of the influence of tectonism (i.e., faulting and hydrologically interconnected jointing) on groundwater flow can lead to nonconservative consideration of flow distances, directions, and rates for groundwater flow pathways.

Basis of Concern:

(1) TSPA-1995 does not consider realistic fault and joint geometry in the analysis of fracture flow.

- Only intra-unit fractures with vertical dips are apparently considered (TSPA-1995, pp. ES-15, ES-25, 9-10), while even the flow dynamics model of Montazer and Wilson (1984) which is used in TSPA-1995 (p. 2-8 and Figure 2.6-1) shows lateral flow intercepted by faults which transmit water across units to the water table.

- An example for inter-unit fracture pathway connectivity through four units is briefly discussed (TSPA-1995, p. 7-16 and Figure 7.4-3). Each unit has a thickness, L, corresponding to the fracture pathway length. The conclusion is drawn that "fracture flow has less of an impact than suspected," but that a greater effect would result from a fault pathway with a more direct connection to the accessible environment. In light of the existence of faults at YM (Simonds et al., 1995), it appears that even this inter-unit fracture pathway example may be nonconservative.

(ii) TSPA-1995 uses the ECM assumption which forces liquid movement to be controlled by matrix permeability.

- The ECM formulation forces liquid movement to occur primarily in the matrix and to be controlled by matrix permeability (with air and vapor movement primarily in fractures and controlled by fracture permeability) (TSPA-1995, p. 4-4).

(iii) TSPA-1995 does not consider moisture movement in fault zones, as was done by Wittwer et al. (1995) from which the TSPA-1995 hydrostratigraphic model was derived. TSPA-1995 considers conceptualization of fracture-matrix flow to be a source of major uncertainty in describing the hydrologic system. In the 2D cross section used in TSPA-1995, taken from the 3D model of Wittwer et al. (1995), boundaries corresponding physically with the Solitario Canyon and Bow Ridge faults are considered to be no-flow boundaries.

- Wittwer et al. (1995) included treatment of role of major faults on distribution and movement of moisture at YM (TSPA-1995, pp. 7-4 and 7-5). They concluded that the hydrological characteristics of major faults are extremely important because fluid flow is strongly influenced by these characteristics, so choice of two major faults as no-flow boundaries in TSPA-1995 may represent a nonconservative conceptual model (although one possible "end-member" model).

(iv) TSPA-1995 does not adequately represent "fast" flow pathways since nonequilibrium fracture flow cannot be represented by the equivalent continuum model (ECM). It is stated in the report (p. 7-9) that better models are needed to describe nonequilibrium fracture-matrix interaction since (p. 7-14) fracture flow through the unsaturated zone can significantly reduce travel time to the accessible environment.

- Forcing fractures to remain dry until the matrix is fully saturated artificially inhibits episodic and rapid movement of water along "fast" fracture pathways (TSPA-1995, p. 7-7). However, it appears that an extra degree of freedom was allowed in sensitivity studies to investigate effects of a relaxed fracture-flow initiation criteria.

(v) TSPA-1995 may impose an artificial limit on the number of WPs which can get wet because of dripping fractures in the drift by not considering how seismotectonic effects possibly influence opening and closing of fractures when time frames are extended beyond 10,000 to 1,000,000 yr (i.e., it appears that wet fractures remain wet and dry fractures remain dry through time in the abstraction). Thus, the calculations presented in TSPA-1995 (see, e.g., ^{237}Np in Table 9.4-1) may limit the effective radionuclide release rates by 50 percent.

- With $f_{drip} = 0.5$, half of the WPs are subjected to dripping from fractures (p. 7-11 and Table 9.4-1). This may artificially limit release of ^{237}Np between time frames of

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100,000 and 1,000,000 yr as the EBS releases for this radionuclide may suggest based on data in Table 9.4-1.

Recommendations:

(i) Consider models with a more realistic fault/joint geometry where some structures are continuous across units and have dips less than 90 degrees. The National Research Council (1996) report on rock fractures and fluid flow strongly emphasized the importance of representing fractures realistically, as soon as possible, when modeling fluid flow and transport in fractured rock.

(ii) Consider alternatives in which flow is controlled by fracture permeability, with fractures cross-cutting units (i.e., inter-unit fractures) rather than confined within units (i.e., intra-unit fractures).

(iii) Consider other representations of flow through major faults.

(iv) Consider alternative approaches where faults are "fast" pathways for flow so that nonequilibrium fracture-matrix interactions can be analyzed.

(v) Consider scenarios in which seismotectonic activity can produce changes in which fractures are dripping by closing/opening of fractures in response to faulting and seismicity such that the entire radionuclide inventory may be affected by water from dripping fractures, even if it occurs only for 50 percent of the WPs at a time.

7.2.5 General Comment—Faulting Effects on Waste Package Performance

Statement of Concern: Effects of renewed faulting on WP performance and fracture flow have not been adequately evaluated. Reactivation of faults could provide fast paths between overlying perched water zones and the repository horizon.

Basis of Concern:

(i) Assumptions about earthquake magnitudes from fault data used in the PSHA study (Wong et al., 1995) may underestimate risks associated with seismicity.

- The effects of seismicity on rockfall in TSPA studies (Gauthier et al., 1995) considered only earthquakes, determined by the authors as capable of rupturing the entire crust, as potentially producing fault displacement in the repository. Lower bounds for such earthquakes were taken randomly between M=6.0 and M=6.5. This lower bound is arbitrary and nonconservative since smaller earthquakes (M=5.7–6.0) are capable of offsets on the order of 10^{-1} m (Wells and Coppersmith, 1994) and, given a shallow earthquake focus, could also rupture the repository.

- The fact that these smaller ruptures do not necessarily rupture the surface does not preclude them from surface or near-surface rupture. Using surface rupture as a criterion for selecting repository-effecting earthquakes in total system performance (Gauthier et al., 1995) is not conservative. Smaller earthquakes may also affect performance especially with regard to enhanced WP degradation (shaking, enhanced roof fall, and direct rupture).

(ii) The conclusion in TSPA-1995 that consequences of potential seismic activity are negligible is based in part on a single expert PSHA (Wong et al., 1995).

- Single expert PSHAs do not contain the proper extent of uncertainty normally observed in multiple-expert PSHAs (see e.g., Savy et al., 1993 and Sobel, 1993). DOE currently plans to conduct multiple PSHA; their results are awaited.

Recommendations:

(i) Estimates of paleoseismicity should be adjusted for the possibility of large undetected earthquakes ($m \leq 6.9$) on blind faults. Smaller magnitude earthquakes should also be considered.

(ii) Perform a multiple expert PSHA following an accepted elicitation procedure and expert selection criteria (see e.g., DeWispelare and Bonano, 1995).

7.2.6 General Comment—Conceptual Tectonic Models

Statement of Concern: Conceptual tectonic models have not been adequately incorporated into TSPA-1995 analyses. Because this has not been done, their effects on performance has not been evaluated.

Basis of Concern:

(i) Representations of faults, distribution of earthquakes, and estimates of faulting parameters were not constrained by viable conceptual tectonic models.

- In the PSHA study of Wong et al. (1995), normal faults were described with assumed planar geometries and dips of either 50, 60, or 70° while strike-slip fault dips were assumed to be planar with dips of either of 70, 80, and 90°. Oblique slip on faults and low-angle (listric or detachment) faults and nonplanar faults with variable dip were not considered.

- A simplified fault geometry based on a random distribution of fault orientations was used to test the occurrence of intersections of primary faults and their associated (secondary) fault zones with the repository. The depiction of fractures and faults in the supporting studies assumed a circular geometry in which faults can have variable strikes. Yet, nearly all faults in the YM region trend north-south or northeast-southwest (e.g., see Faulds et al., 1994). Conclusions drawn from the performance studies summarized in Gauthier et al. (1995) may not be at all representative of repository performance when a more realistic representation of faults is assumed.

(ii) Tectonic models are needed to develop and evaluate assumptions about expected future seismicity.

- If Crater Flat is modeled as a modified pull-apart basin (Fridrich et al., 1994) for example, then multiple fault rupture due to a large magnitude earthquake may become significant. In this model, numerous large-magnitude earthquakes (M >7.0) rupture multiple and complex fault segments, which by their individual lengths, would not seem to support such large-magnitude events.

- Analog modeling results (Stamatakos and Ferrill, 1996) as well as recent field evidence (e.g., DePolo, et al., 1991; Zhang et al., 1989) suggest that multiple-rupture plane earthquakes become more likely as pull-apart basins mature.

(iii) Conceptual tectonic models are also critical for assessing the likelihood of linked faulting (e.g., where slip on a master fault results in significant compensatory slip on subordinate faults) or clustered seismic activity (e.g., changes in crustal stress due to rupture of a fault in the far-field triggers rupture on remote faults.

- The Little Skull Mountain aftershock was part of a clustered seismic event that was triggered by the Landers earthquake. Fault geometries that more accurately reflect the structural framework of the YM region need to be used.

Recommendations: Faulting parameters and estimates of future seismicity used in total system performance analyses need to be assessed within the context of viable tectonic models of the YMR. The models that DOE chooses to use in support of a License Application should reflect the range of models that can be constrained by the data. The DOE should justify the exclusion of models that may lead to higher releases. This will provide greater confidence that the nature frequency and magnitude of seismic events, tectono-magmatic interaction, and effects of tectonics on groundwater flow have not been underestimated.

7.2.7 General Comment—Pre-Existing Fractures and Thermal Loading

Statement of Concern: Orientation of pre-existing fractures in the present-day stress field was not considered in determining whether thermal loads induce the opening or closing of near-field vertical fractures. The hydraulic characteristics of fractures in the near-field will determine the rate of water flow into and out of the repository.

Basis of Concern: TSPA-1995 does not mention fracture orientation in the discussion of whether near-field vertical joints may open or close due to the horizontal compressive stress induced by application of thermal load.

- Based on information in an M&O letter report it is stated in TSPA-1995 that near-field vertical joints above and below the drift may close due to horizontal compressive stress induced by thermal loading of the rock mass, while near-field horizontal joints may open as much as 0.2 mm (TSPA-1995, p. 4-15). It was acknowledged that this response to thermal loading could affect bulk permeability (and, hence, conductivity) in the near-field, and may exceed the strength of the rock mass. It was concluded that thermal-mechanical coupling may need to be included in subsequent TSPA iterations.

Recommendation: Consider the importance of orientation of pre-existing vertical fractures and the present-day stress field for analyzing whether vertical fractures may selectively open or close in response to thermally induced horizontal compressive stress. Factor this information into determination of potential effects on near-field bulk permeability and conductivity.

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8 KEY TECHNICAL ISSUE: EVOLUTION OF NEAR-FIELD ENVIRONMENT

8.1 SCOPE OF REVIEW

The portions of TSPA-1995 relevant to the KTI concerning characterization of the evolution of the near-field groundwater chemistry in unsaturated media, transient thermal conditions, uncertain fluid fluxes, and uncertain thermodynamic characteristics of materials are identified in Table 8-1.

Table 8-1. Total System Performance Assessment 1995 scope of review for the Key Technical Issue: Evolution of Near-Field Environment

Section	Title
4.5	Thermal-Chemical Effects in the Near-Field Environment
6.2	Waste Form Alteration Modeling (shared with Container Life and Source Term KTI)
6.3	Solubility-limited Aqueous Radionuclide Concentrations
6.4	Colloid Contributions to Mobile Mass of Radionuclides

8.2 GENERAL COMMENT—NEAR-FIELD CHEMISTRY

Statement of Concern: Possible geochemical variations in near-field environmental conditions are considered reasonably well in TSPA-1995, Chapter 4. However, minimal effects of changes in the geochemical environment are employed in the performance calculations.

Basis of Concern: With regard to solubilities it is stated, "Because the actual changes to the near-field environment are not yet well-defined, incorporation of such effects either into [solubility] distributions such as those discussed above or into models for predicting the solubility-controlling phases for each radionuclide is not currently possible" (p. 6-11). Although some pH dependent solubility relations were derived (TSPA-1995, Eqs. 6.3-1 to 6.3-3), it was concluded that, "Although the derived functions incorporate pH-dependence explicitly, the near-field pH evolution is uncertain to the extent that adequate constraints do not exist for making a pH choice other than a random selection from a distribution" (p. 9-25). For alternate solubility models (TSPA-1995, Section 9.3.6) only pH 7 was considered, which conflicts with the statement "These results are used to evaluate the release of these radionuclides based on explicit dependence for both pH and temperature" (TSPA-1995, p. 6-6).

In general, solubilities used in TSPA-1995 are highly uncertain, which is partly represented by distributions spanning many orders of magnitude (TSPA-1995, Figures 6.3-1 to 6.3-17). Comparisons to solubilities for selected elements determined in preliminary independent computations using EQ3NR (version R2; com data set; Wolery, 1992) for ranges of possible geochemical conditions revealed that most TSPA-1995 solubilities are comparable or higher (more conservative). Two exceptions are radium (Ra) and tin (Sn). Calculated solubilities of $RaSO_4$ and cassiterite (SnO_2) for a range of possible water chemistries and temperatures were near 10^{-6} molal. This value is near the upper limit of the TSPA-1995 range for Ra and 10 times the upper limit of the TSPA-1995 range for Sn. However, considering $RaSO_4$ or SnO_2 to limit solubility is perhaps unnecessarily conservative because these trace metals are likely to be incorporated as minor components of other phases. The EQ3NR results are also subject to large uncertainties because of uncertain thermodynamic data and environmental characteristics. It appears that the authors of TSPA-1995 recognize the significance of near-field geochemistry and its complexity. Nevertheless, near-field chemistry and its likely variations were not considered explicitly in selecting solubilities.

Recommendations: It is recommended that geochemical models be developed for the near-field geologic setting and the engineered barrier system and that solubilities used for the source term account for dependencies on pH, carbonate, ionic strength, temperature, and other important parameters. This effort will also aid in addressing issues raised in Section 6 with regard to container life and source term.

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9 KEY TECHNICAL ISSUE: RADIONUCLIDE TRANSPORT

9.1 SCOPE OF REVIEW

The portions of TSPA-1995 relevant to the KTI concerning processes which may affect radionuclide transport from the repository to the accessible environment are identified in Table 9-1.

Table 9-1. Total System Performance Assessment 1995 scope of review for the Key Technical Issue: Radionuclide Transport

Section	Title
6.5	Radionuclide Transport Modelling
7.4.6	Radionuclide Retardation

9.2 GENERAL COMMENTS—SORPTION AND DIFFUSION

9.2.1 General Comment—Radionuclide Retardation

Statement of Concern: Radionuclide retardation is a complex coupling of different processes that are all strongly affected by system chemistry. To address uncertainties in retardation, a range and distribution of sorption coefficients (K_d) is assumed in TSPA-1995 for radionuclide transport through the unsaturated and saturated zones. In both the saturated and unsaturated zone, retardation appears to be limited to matrix transport only. Few details are provided on the informal elicitation procedure used to develop the PDFs, and no clear technical basis is identified to justify the ranges and distributions selected for a given sorption coefficient. It is therefore not clear whether the PDFs as presented take into account the entire range in pH and solution chemistry that may be relevant to radionuclide retardation at YM. It is therefore not clear that the approach taken is in all cases conservative or bounding.

Basis of Concern: The model for the unsaturated zone consists of three "rock types:" devitrified tuff, vitric tuff, and zeolitized tuff. The saturated zone is modeled only as devitrified tuff. The K_d values for the saturated zone are essentially identical to those given for the unsaturated zone, with higher values given for Pu, U, Np, Ra, and Sr attributed to higher ionic strength in the unsaturated zone waters. It is not clear from the discussion which units are considered devitrified, vitric, and zeolitic, and therefore not clear whether this division of rock types is appropriate. TSPA-1993 (Wilson et al., 1994) offers a correlation between hydrogeologic units and rock types, but it is not stated if this has been adopted in TSPA-1995.

DOE recognizes the limitations of the K_d approach (e.g., Reardon, 1981; Nuclear Regulatory Commission, 1989) due to its simple representation of retardation processes such as precipitation/dissolution, ion exchange, sorption, and surface complexation (TSPA-1995, p. 7-20). An additional uncertainty is in using empirical parameters derived from lab scale batch sorption experiments to represent retardation in field-scale transport calculations. PDFs are based on experiments performed at ambient temperatures (~25 °C) which may not be appropriate, given likely temperature perturbations due to the emplacement of waste.

No information is provided on the source of the K_d ranges except reference to a memorandum (Meijer, 1995) and the TSPA-1993 discussion (Wilson et al., 1994, Chapter 9). Np, U, and Pu sorption data can be traced to LANL reports, but other sources of radionuclide sorption data are not referenced. Few details are provided on the elicitation procedure used to derive the different PDFs, and no clear mechanistic relationship is identified to justify the ranges selected for the sorption coefficient. It is not clear whether the PDFs as presented take into account the entire range in pH and chemistry that may be relevant to retardation at YM. It is therefore not clear that the approach taken is conservative or bounding.

Because K_d is a derived parameter that depends on system chemistry in a different way for each radionuclide, random selection from K_d ranges does not adequately express chemistry effects or correlations that exist between different elements. For example, at low pH both Pu and Ni sorption on simple oxides are low. Random sampling on K_d ranges that do not consider this pH relationship, however, may result in high Pu and low Ni sorption. For TSPA-1993, Wilson et al. (1994) developed a rank correlation between elements that behave similarly. It is not clear whether this correlation can address the different processes contributing to sorption, or whether this or any other type of correlation has been adopted in TSPA-1995. The absence of such considerations makes it likely that some TSPA-1995 results are internally inconsistent and not chemically reasonable.

Recommendations: A more thorough documentation of assumptions is needed. The elicitation process should be formalized, and the reasoning used in establishing the PDFs should be explicitly defined. Correlation among radionuclides with regard to sorption behavior needs to be defined and/or strengthened. Perhaps a better approach would be to develop models that reflect the effects of system chemistry, and then use chemical variables that can be measured in the field such as pH and PCO_2 as TSPA sampling parameters.

9.2.2 General Comment—Matrix Diffusion

Statement of Concern: The description of the treatment of matrix diffusion misrepresents the effects of matrix diffusion.

Basis of Concern: It is stated on TSPA-1995, Page 9-23 "In the extreme case of equilibrium matrix diffusion (Golder, 1993), the solutes in fractures would travel at the same velocity as solutes in the matrix, and the effect would be the same as having matrix-flow-only, i.e., zero fracture flow. Thus, although we have not modeled matrix diffusion, per se, in TSPA-1995, Figures 9.3-49 and 9.3-52 show its maximum effect on the model." This conclusion is difficult to understand. It is conceivable that "equilibrium matrix diffusion" is intended to describe the case where matrix concentrations have equilibrated with fracture concentrations due to fast diffusion. However, the relation to relative rates of fracture flow and matrix flow is unclear. Perhaps it was reasoned that because diffusion is generally slow, the fracture flow rate must be negligibly different from the matrix flow rate for fracture compositions to equilibrate with matrix compositions. This condition may represent an extreme of matrix diffusion effects, but it is the least conservative extreme. The conservative extreme of matrix diffusion effects would be all

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transport in fractures and zero concentrations in the matrix, which was not modeled. The rationale for having implicitly examined matrix diffusion effects appears to be flawed. Rapid flow in fractures and lack of chemical equilibrium between fractures and matrix (e.g., Fabryka-Martin et al., 1996) also suggest that matrix diffusion would be an important process affecting radionuclide transport from the repository.

Recommendations: A logical recognition of the role of matrix diffusion should be provided, and assessed in evaluations of radionuclide migration in the absence of fracture-matrix equilibrium.

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10 KEY TECHNICAL ISSUE: REPOSITORY DESIGN AND THERMAL MECHANICAL EFFECTS

10.1 SCOPE OF REVIEW

The portions of TSPA-1995 relevant to the KTI concerning the design of the repository and the effects of thermal-mechanical coupled processes are identified in Table 10-1.

Table 10-1. Total System Performance Assessment 1995 scope of review for the Key Technical Issue: Repository Design and Thermal Mechanical Effects

Section	Title
3.1	Introduction
3.2	General Layout Considerations
3.3	Thermal Loading Issues
3.4	Layouts for 25 and 83 MTU/Acre
3.6	Waste Package Emplacement
4.2	Drift-Scale Thermal-Hydrology
4.4	Near-Field Thermal-Mechanical Considerations

10.2 GENERAL COMMENTS—REPOSITORY CHARACTERISTICS

10.2.1 General Comment—Thermal-Mechanical Coupled Response

Statement of Concern: DOE (TSPA-1995, p. 1-4) has acknowledged that the thermal-mechanical response of the rock mass surrounding the emplacement drifts and associated changes in the near-field hydrology may affect repository performance. However, DOE has not included the thermal-mechanical coupled response into predicting system performance by assuming that the coupled effect is probably insignificant as the variability in ambient hydrologic properties accounted for in the analyses would encompass the increase in hydraulic conductivity expected as a result of the coupled effect. DOE has not provided adequate justification for this assumption.

Basis of Concern: Evaluation of pre- and post-closure performance requires an understanding of the thermal-mechanical response of the jointed rock mass as it impacts the drift stability, retrievability of WPs, near-field environment and WP degradation, performance of seals, and flow and radionuclide transport. The long design life requires a consideration of the thermal-mechanical effects on the stability of drift openings, changes of rock properties with time in the repository environment, and uncertainties in the useful life of the installed support systems under the repository environment.

Maintaining the retrievability option requires the drift openings to be stable until permanent closure (a minimum of 100 yr). During the retrieval period, thermal stresses resulting from the emplaced waste will be very high (TRW Environmental Safety Systems Inc., 1994; M&O, 1995). The tangential stresses at the roof or floor of the excavation may reach 73 MPa for a heat load of 83 MTU/acre. Under the high state of stresses, the underground excavations are expected to be less stable. The uniaxial compressive strength of the TSw2 unit varies from 32 to 290 MPa with an average of 160 MPa (Department of Energy, 1994). TSw2 unit rock mass can withstand an ultimate principal stress at failure of 49 MPa with a confining pressure of 7 MPa (Department of Energy, 1994). These observations suggest overstressing and local failure could occur around the emplacement regions.

Excavations subjected to repetitive episodes of seismic motions, as expected during the long life of a repository, may fail due to accumulation of shear damage along the fractures at a peak particle motion relatively smaller than the probable maximum value (Brown and Hudson, 1974; Barton and Hansteen, 1979; Hsiung et al., 1992; Kana et al., 1995). Therefore, the possibility of coalescence of relatively small failure zones leading to a large failure zone remains a distinct possibility. During the containment period (up to 1,000 yr), thermal-mechanical interactions in the rock mass surrounding the drifts and the resulting changes in the near-field hydrology may have an impact on the performance of the WPs and flow and radionuclide transport processes at the repository (National Research Council, 1996; Ahola et al., 1993). Rock falls initiated by unstable drift roof and sidewalls could have an impact on the WP performance. Furthermore, seismically induced rock falls could, depending upon the design (e.g., emplacement drifts not backfilled after permanent closure), contribute to local acceleration of WP degradation, resulting in an early loss of containment or an increased release rate.

After permanent closure, microfractures will develop in the rock matrix as a result of the creep process. This could lead to an increase in porosity which, in turn, increases the permeability (Martin et al., 1995; Takahashi et al., 1991). Moreover, it is expected that the creep will be more prevalent on joints. Under this weakened condition, the rock mass will be even more susceptible to repetitive seismic loads, resulting in further accumulation of joint deformation. This accumulation could potentially modify the preferential flow paths in the rock mass surrounding the emplacement horizon (Raney, 1988).

Fractures or joints dilating due to thermal-mechanical interactions may impact flow and transport at the site, and hence, may be significant to the performance of the repository (Makurat et al., 1990). Moisture from condensate regions and perched water zones above the repository can travel quickly to the emplacement region through such preferential flow paths (Buscheck and Nitao, 1993).

A simplified analysis (M&O, 1995) shows that the increase in hydraulic conductivity caused by thermal-mechanical interaction is about three orders of magnitude. It is noted that this increase in hydraulic conductivity is an increment to the *in situ* hydraulic conductivity and should be considered in addition to the natural variability of hydraulic conductivity at the site.

Recommendation: DOE should justify the assumption that the thermal-mechanical coupled effects are insignificant. Otherwise, additional analyses should be made considering the potential for increased flow in the near-field environment to assess impacts on total system performance.

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10.2.2 General Comment—Adequate Characterization of Optional Repository Areas

Statement of Concern: DOE has acknowledged that if the low thermal loading strategy (25 MTU/acre) is adopted, three additional emplacement areas, Optional Areas B, C, and D, will be required to provide adequate room for 63,000 MTU of spent nuclear fuel. The TSPA-1995 for the low thermal load of 25 MTU/acre assumes important site characteristics such as infiltration rate, hydraulic properties, and dilution characteristics to be similar to those of the primary disposal block used in the TSPA for the high thermal load of 83 MTU/acre.

Basis of Concern: Additional emplacement areas required for 63,000 MTU of spent fuel, namely, Optional Areas B, C, and D, are quite far away from the ESF facility, as shown in Figure 3.4-1 of TSPA-1995. For example, Optional Area D may be 2 to 3 kilometers away from the ESF. As recognized by the M&O (1993), the IGIS model for geologic data for the TSw2 thermomechanical unit does not extend that far from the potential primary emplacement region. Consequently, available geological information on the characteristics of the repository horizon in these optional areas may not be sufficient and the studies carried out to characterize the repository horizon may not adequately characterize these areas.

Recommendation: DOE needs to provide a plan for characterization of these optional areas if the low thermal load is selected.

10.2.3 General Comment—Seals

Statement of Concern: TSPA-1995 does not address seals. No justification is provided for this assumption.

Basis of Concern: Seals may be important components in the repository design for providing a barrier to radionuclide migration along preferred pathways introduced by drilling and construction.

Recommendation: DOE should consider the effect of seals in the next revision of the TSPA.

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