February 19, 1997

Ronald A. Milner, Director
of Program Management and Integration
Office of Civilian Radioactive Waste Management
U.S. Department of Energy
1000 Independence Avenue, SW
Washington, DC 20585

SUBJECT: RETRANSMITTAL OF THE CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES DETAILED REPORT RELATED TO THE AUDIT REVIEW OF THE U.S. DEPARTMENT OF ENERGY'S 1995 TOTAL SYSTEM PERFORMANCE ASSESSMENT

Dear Mr. Milner:

By letter to you dated November 5, 1996, I believed that I transmitted to you, and those on the normal distribution list, the above-referenced report. Several on the distribution list apparently did not receive the report. Therefore, I am retransmitting it but, in future references to that report, we will cite the November 5, 1996, letter as the reference for circulation of the report.

If you have any questions regarding this letter, please do not hesitate to contact me on (301) 415-7252.

Sincerely,

[Original signed by:]

John H. Austin
Performance Assessment and High-Level
Waste Integration Branch
Division of Waste Management
Office of Nuclear Materia Safety
and Safeguards

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TOTAL SYSTEM PERFORMANCE ASSESSMENT 1995 AUDIT REVIEW

Prepared for

Nuclear Regulatory Commission
Contract NRC-02-93-005

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1 INTRODUCTION

1.1 BACKGROUND

The U.S. Department of Energy's (DOE) third total system performance assessment (TSPA) for the proposed high-level waste (HLW) repository at the Yucca Mountain (YM) site is documented in the report entitled "Total System Performance Assessment—1995: An Evaluation of the Potential Yucca Mountain Repository" (TRW Environmental Safety Systems, Inc., 1995a). The report, referred to herein as TSPA-1995, presents the DOE performance assessment (PA) approach, assumptions, data, calculation results and principal conclusions 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. The results of the review consist of technical concerns developed by the NRC with support from the Center for Nuclear Waste Regulatory Analyses (CNWRA). These concerns, which are detailed in Section 1.5, formed the basis for discussions at the NRC/DOE Technical Exchange Meeting, May 22-23, 1996. The review also identified additional topical areas to be investigated during the detailed review which is scheduled to be completed in December 1996. The detailed review will not only include these additional areas, but will also attempt to determine and describe the significance to performance of all NRC staff concerns. Issues will be investigated only to the extent that they continue to demonstrate significance to performance.

1.2 OBJECTIVES OF THE AUDIT REVIEW

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): (i) Total System Performance Assessment and Technical Integration, (ii) Igneous Activity (Volcanism), (iii) Unsaturated and Saturated Flow Under Isothermal Conditions, (iv) Thermal Effects on Flow, (v) Container Life and Source Term, (vi) Structural Deformation and Seismicity, (vii) Evolution of the Near-Field Environment, (viii) Radionuclide Transport, (ix) Repository Design and Thermal-Mechanical Effects, and (x) Support Development of the EPA Standard and NRC Regulation. Each of the above KTIs encompasses a number of subissues that NRC uses to guide its program and resolution of the principal issues.

These KTIs were identified through a combination of:

- Iterative performance assessment (IPA)

- A systematic regulatory analysis of the Code of Federal Regulations (CFR) Title 10, Part 60 (10 CFR Part 60)

- NRC staff understandings of geologic processes and events relevant to the YM site.

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).

1.4 REVIEW APPROACH

The DOE TSPA-95 offers a more complete and comprehensive analysis of undisturbed repository performance than previous TSPAs. In addition, TSPA-95 has built upon the experience of prior TSPAs and has added more mechanistic processes to help reduce uncertainty. In contrast to previous audit reviews of DOE TSPAs, NRC has selected, for this review, very specific topical areas considered to be of key importance to the determination of total system performance. For this audit review, five primary topics were selected for more extensive evaluation by NRC and CNWRA staffs and are discussed within this report:

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

Audit review findings concerning the remaining KTIs (and subissues) will be evaluated in detail in the December 1996 report.

The five focus topics were selected because of their importance to the developing DOE WCIS, as well as NRC/CNWRA determinations of significance to performance from the IPA Program. An additional consideration in the selection of topical areas was to evaluate areas where the NRC and CNWRA staffs have performed sufficient technical analyses to independently evaluate DOE's analysis.

Within these five topical areas, the DOE TSPA methodology presented in TSPA-1995 was reviewed with respect to appropriateness of the technical approach (i.e., conceptual and mathematical models), adequacy of the treatment of uncertainties, use of conservative assumptions, sufficiency of site data, and consistency with previous DOE TSPAs. Supplemental, independent calculations were made by NRC/CNWRA staff to the extent feasible through the conjunctive use of simple and detailed process models, as well as the NRC IPA Phase 2 Total Performance Assessment (TPA) computer code (Nuclear Regulatory Commission, 1995). These audit review analyses are intended to help DOE better understand NRC approaches that will be used in compliance determination.

1.5 REFERENCES

Federline, M.V., R.L. Johnson, and J.T. Greeves, "NRC's Refocused Prelicensing High-Level Waste Regulatory Program," *Proceedings of the High-Level Radioactive Waste Management Conference*, Las Vegas, Nevada, 1996.

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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 TSPA
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 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 TPA code [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 these CCDF results requires independent calculation.

2.2.2 Description of Department of Energy Approach and/or Position

In 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 expressed in terms of CCDF for comparison with the total-system performance standards in 10 CFR 60.112. DOE selected RIP as its total-system performance computer code mainly as a result of: (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 (TRW Environmental, 1995).

The RIP code consists of four main component models: (i) waste package behavior and radionuclide release from the EBS (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 arbitrary assumptions were used in selecting the parameter ranges and distributions. In TSPA-1995, the assumptions used were often not properly justified or supported by available data. For example, the effective porosity in the unsaturated zone was assumed to be .0001 (which is representative of fracture porosity) for all strata, whereas for the saturated zone, an effective porosity of 0.2 (which is representative of matrix porosity) appears to have been 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 (Domenico and Schwartz, 1990; Erickson and Waddell, 1985). Erickson and Waddell, (1985) estimated fracture porosities of the productive zones in the tuff aquifer to range from about 10^{-4} to 10^{-3}.

2.2.3 Description of Nuclear Regulatory Commission Approach and/or Position

The NRC developed the TPA computer code (Sagar and Janetzke, 1993) 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 CCDFs 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. The executive module controls the manner and sequence in which the modules containing the different models and algorithms within TPA are executed. The executive model also controls the transfer of data among the various TPA modules. 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.

The approach used in this audit review of TSPA-95 consisted of applying the IPA Phase 2 version of TPA in the following manner:

- Use a digitized canister lifetime cumulative distribution function (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.

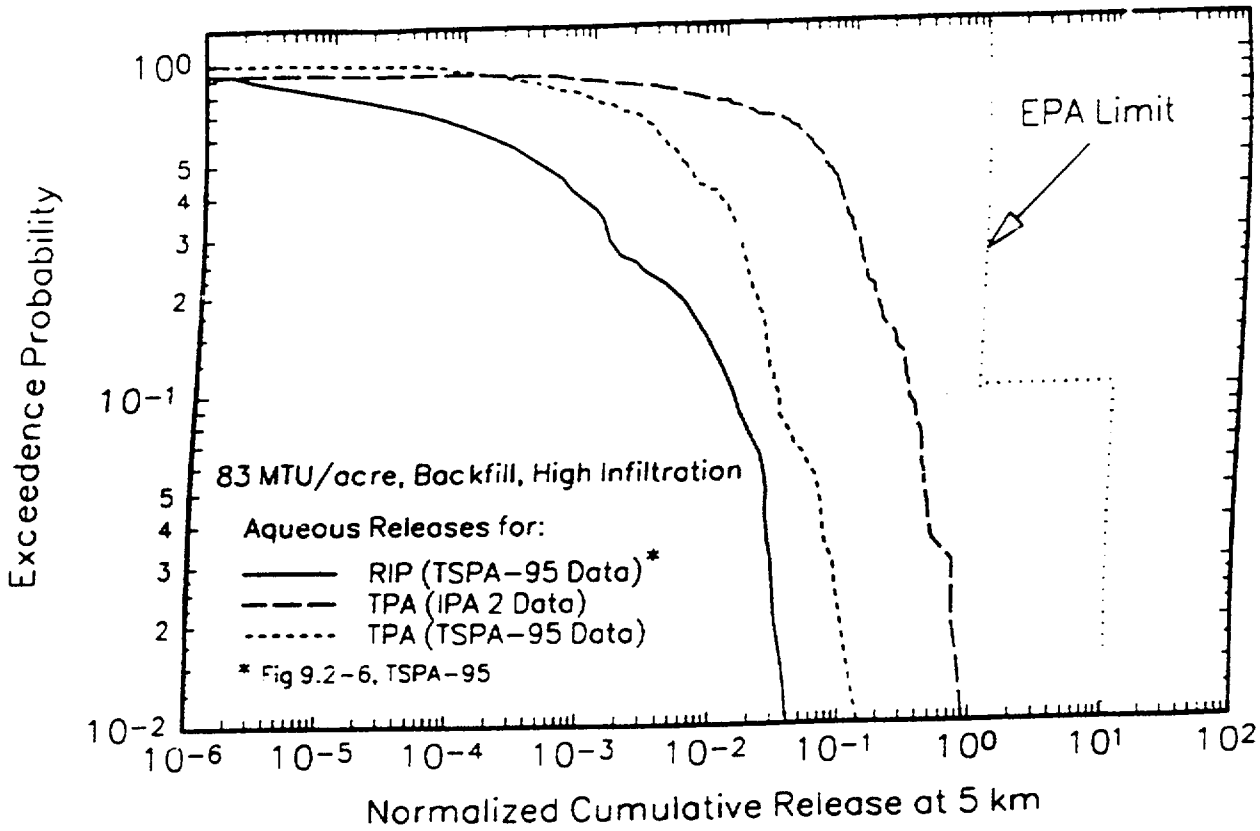


Figure 2-1. Comparison of CCDFs for cumulative release of liquid phase radionuclides

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 selected for this analysis. That figure gives the cumulative fraction of failures (by various corrosion processes) for various exposure times. The CDF was digitized and a histogram constructed. The canister lifetime curve was calculated by RIP for the following canister conditions: thermal load of 83 MTU/acre, high infiltration, backfill, and relative humidity (RH)-dependent corrosion initiation. Two CCDFs independently computed with TPA 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 set (modified only for consistency with new waste package design) and the digitized TSPA-1995 canister lifetime curve, and (ii) the approximate representation of TSPA-1995 data set and the digitized TSPA-1995 canister lifetime curve.

In the first case, the TPA (IPA Phase 2 data) CCDF is below the U.S. Environmental Protection Agency (EPA) limit with small compliance margin, 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 agree well with the RIP calculations for low releases; however, the TPA results indicate a higher frequency of larger releases than indicated by the RIP results. This suggests that some of the IPA Phase 2 assumptions and site subsystem abstractions are more conservative than those used in RIP. For example, in the TPA calculations it was assumed that once a canister failed in a given zone of the repository, all canisters within that zone failed, a more conservative assumption than that used in TSPA-1995. In the second case,

the TPA (run with TSPA-1995 data) results show a large compliance margin but overall high releases than the RIP CCDF.

The residual differences between the TPA and RIP CCDFs are probably the result of differences in abstracted models and conceptual representation of the system. The major differences between the two independently calculated CCDFs and the selected CCDF from TSPA-1995 were hypothesized to be the result of different (i) methods for calculating particle travel times through the unsaturated zone, and (ii) representations of the hydrostratigraphy of the unsaturated and saturated zones.

To evaluate the first of these hypotheses, the distributions of particle travel times were computed using both TPA and RIP methods. These calculations, performed with the MatLab software, produced CDFs for the particle travel time which are compared in Figure 2-2. The TPA model abstraction and data better capture the effects of both fracture flow (i.e., fast pathways) and matrix flow behavior, whereas the RIP model abstraction (and input data) lacks an adequate representation of fracture flow.

To investigate 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 models differ in that: (i) the Topopah Springs unit is subdivided into vitric (TSv) and welded (TSw) components in the TSPA-1995 model and (ii) the Calico Hills nonwelded zeolitic (and low permeability) subunit and the Calico Hills non-welded vitric (CHnv) subunit are present in all ten of the TSPA-1995 pathways, in contrast to the IPA 2 model, where they are each absent in two of the seven pathways (subzones). The longer path length and lower effective conductance of the flow path explains to a large degree the longer particle travel times computed in TSPA-1995. The absence of short particle travel times or fast pathways in the TSPA-1995 is 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.

2.2.4 Description of Likely Effects on Performance

The calculation of CCDFs that are both representative and consistent is critical in the determination of overall repository performance. Audit review results indicate significant differences between CNWRA/NRC and TSPA-95 calculated CCDFs due to differences in basic methodology. In general, the abstracted models and conceptual representation of the system used in RIP are less conservative than those incorporated in TPA, leading to an underestimate of the effects of fast pathways and an underestimation of cumulative releases. Comparisons of TSPA-95 and CNWRA/NRC independently calculated results for drinking water dose indicate a significantly delayed and reduced dose in TSPA-95 results (see Appendix A). The Markovian model of matrix diffusion used in TSPA-95 calculations appears to provide for longer radionuclide migration times than may be justifiable (see Appendix B).

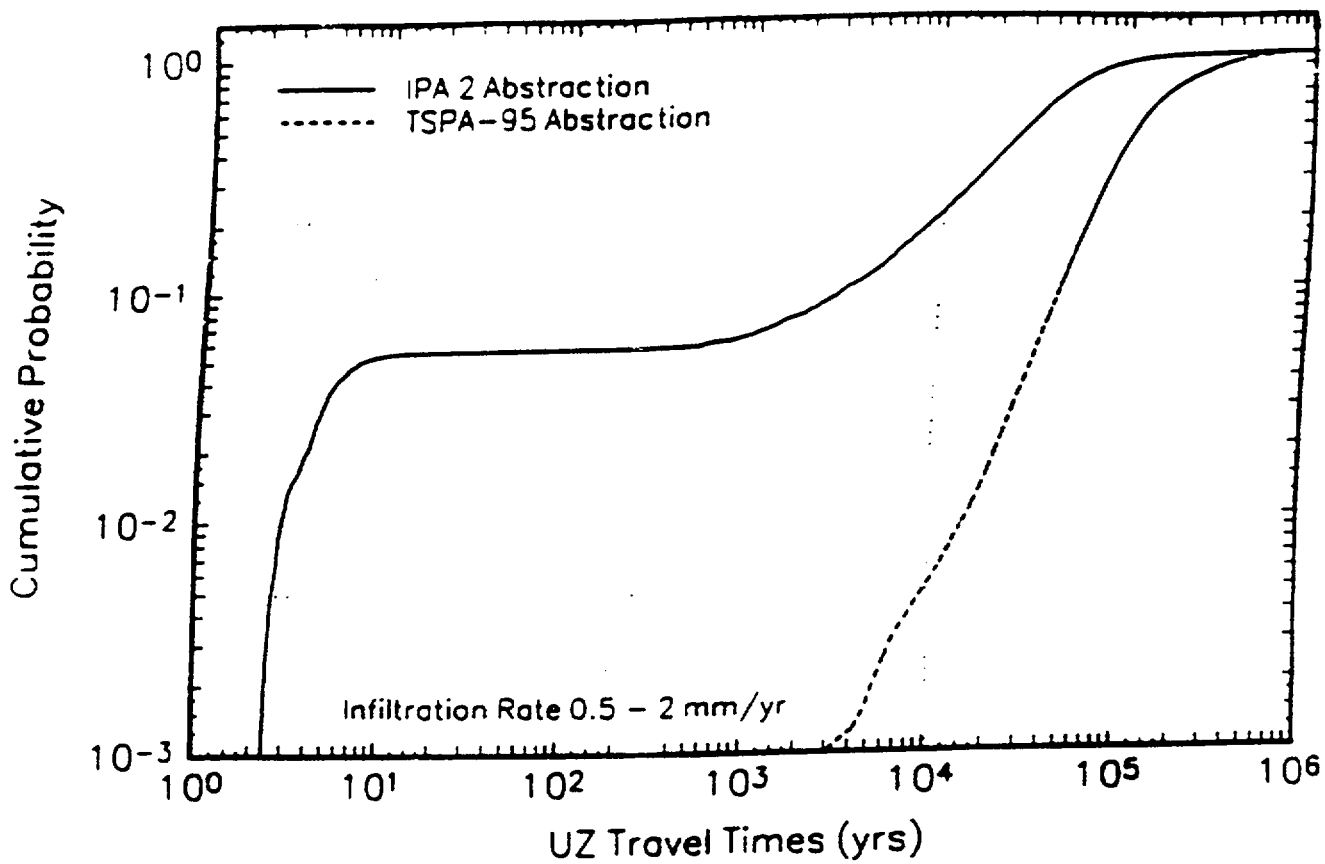
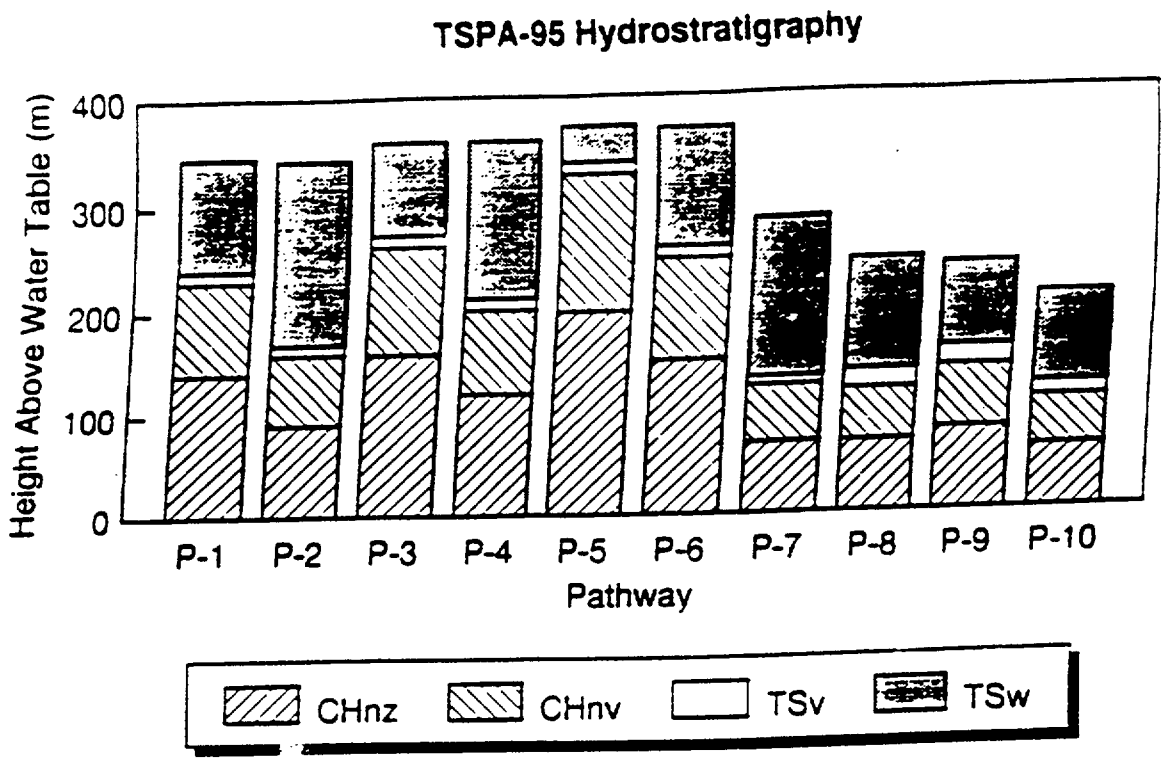


Figure 2-2. Comparison of CCDFs for particle travel-time

Additional evaluation is needed to fully delineate the factors producing the differences in the CCDFs and to improve both the NRC and DOE approaches and data sets. The DOE approach needs to better reflect the fast paths which are consistent with the hydrogeology of the YM site and with interpretations of recent chlorine-36 data (Fabryka-Martin et al., 1996). The NRC approach needs to: (i) utilize an updated representation of the hydrostratigraphy, (ii) utilize regular discretization, and (iii) examine the possibility that assumptions associated with canister failures in repository subzones.



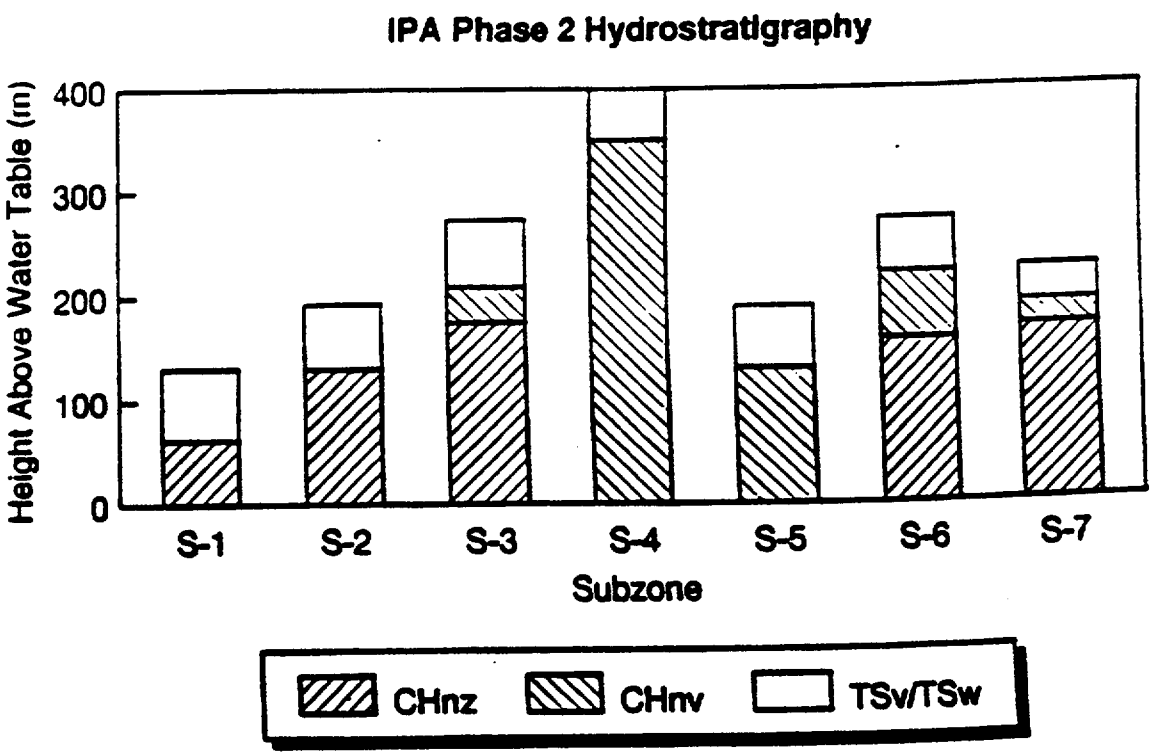


Figure 2-3. Comparison of hydrostratigraphic models

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

3.1 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 isothermal conditions are identified in Table 3-1.

Table 3-1. 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
2.6	Unsaturated Zone (UZ) Hydrology
3.8	UZ Pathway Stratigraphy
7.1	Introduction
7.2	UZ Ambient Hydrology
7.3	Drift Scale Hydrology
7.4	Unsaturated Zone Transport (shared with Radionuclide Transport KTI)
7.6	Saturated Zone Transport (shared with Radionuclide Transport KTI)
7.7	Climate Change

3.2 AREA OF CONCERN: INFILTRATION

3.2.1 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 consequent impacts on WP degradation and radionuclide transport rates through the unsaturated zone. Infiltration rates are assumed to control percolation fluxes and 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)
- Fracture-flow velocities not adjusted for water saturation level
- 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

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

In 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 an assumed fracture continuum. Variations of infiltration rates due to climatic changes are 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.

For the "mountain scale" model, flow is assumed to be vertical, with each stratigraphic layer modeled as homogeneous (i.e., fracture properties do not vary between layers or realizations). In each stratigraphic layer, the matrix velocity and the fraction of flow in the fracture continuum is constructed as a function of the areal-average infiltration flux, with maximum and minimum values calculated for 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 utilized in the transport simulation is assumed to be uniformly distributed between the maximum and minimum values, while a log-uniform distribution is assumed for the matrix velocity.

For the "drift scale" model, 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 areal-average infiltration flux values, 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 to calculate 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.

3.2.3 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 include a 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 allows for up to 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. It is not clear that the TSPA-1995 approach is conservative in that the period of regulatory interest is 10 ka. 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 between releases and 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-flow velocity (V_m), fracture-flow 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.

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

The implementation of the abstraction process may be conservative insofar as it is guaranteed that there is some flux in fractures from the repository directly to the water table 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 layers, and the slowest pathway would typically consist of matrix flow through each layer. It is assumed that particles may switch between matrix and fracture only at layer interfaces.

The two extreme flux rates considered in the TSPA-1995 abstraction process, 2 mm/yr and 0.01 mm/yr, are considered in Figures 3-1 and 3-2, respectively. The 12 curves presented in Figures 3-1 and 3-2 represent a matrix, where the line style (dotted, solid, dash-dot) represents the pathway and the symbol style denotes the procedure used to generate the pathways. These figures present the fastest, slowest, and largest-flux pathways for each of 50 process-level realizations, as well as 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) and adapted to incorporate the equivalent continuum model used in the TSPA-1995 abstraction.

Examining the behavior of the 2 mm/yr case in Figure 3-1, 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 indicates a minimum of 200 yr for the fastest pathways, but more typically on the order of 1,000 yr. The 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 rather than [illegible] material property realizations has the effect of making the fastest pathways faster and the slowest pathways slower.

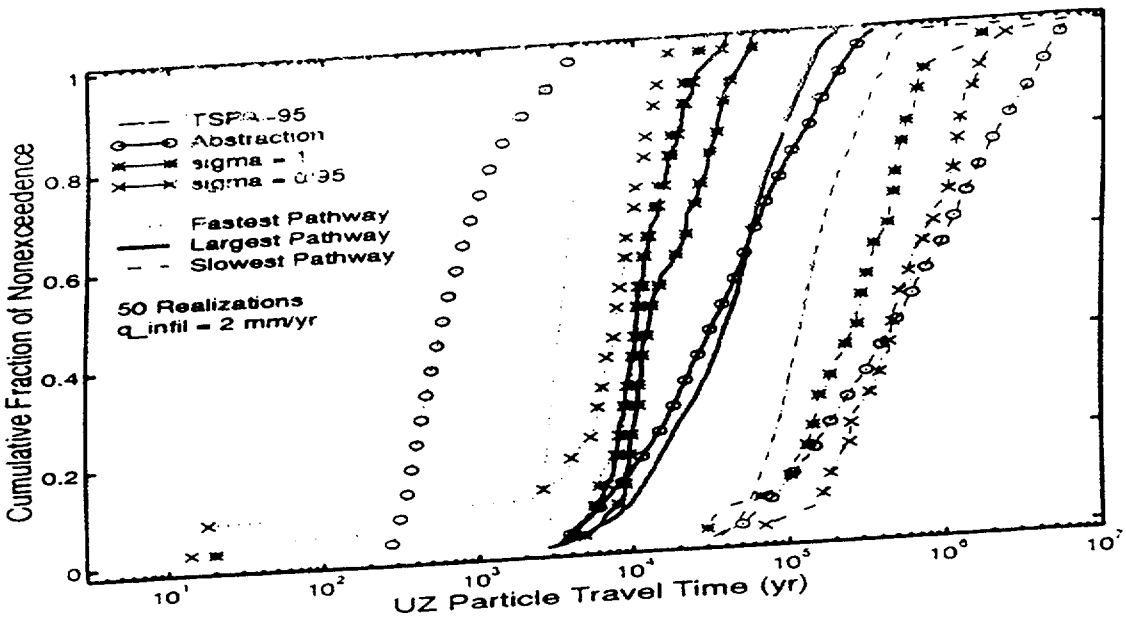

Figure 3-1. Comparison of process-level simulations with abstractions for an infiltration flux of 2 mm/yr

Examining the behavior of the 0.01 mm/yr case in Figure 3-2, 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. Assuming matrix only flow, preliminary 2D vertical-slice simulations using BIGFLOW (Ababou and Bagtzoglou, 1993) suggest that focused infiltration can have a significant impact on fluxes past the repository. This point is demonstrated in Figure 3-3, which shows the impact that localizing

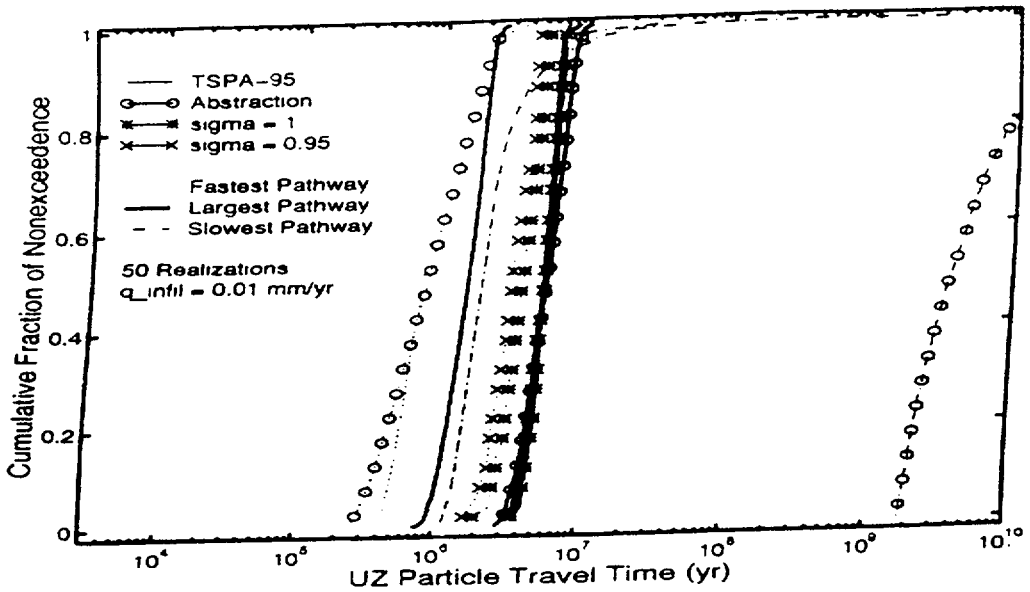

Figure 3-2. Comparison of process-level simulations with abstractions for an infiltration flux of 0.01 mm/yr

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.

3.2.4 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 and will play a central role in determining compliance with the expected risk- or dose-based standard.

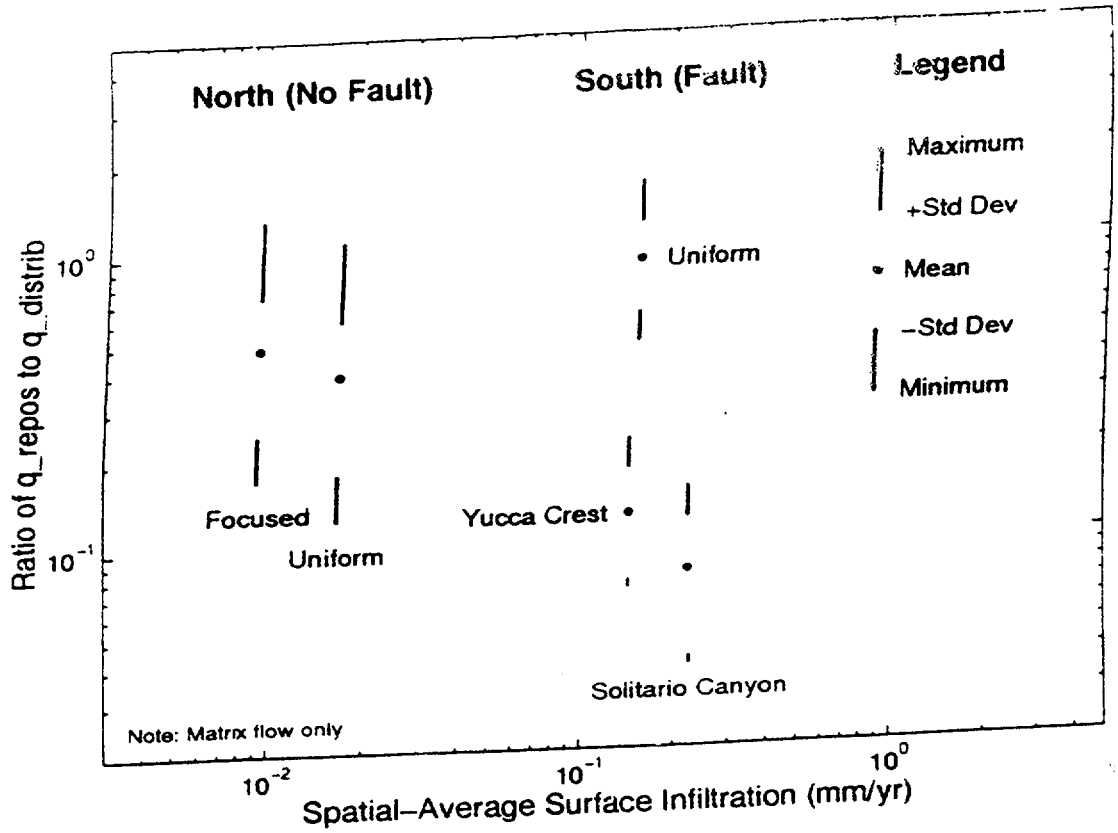

Figure 3-3. Statistical description of element fluxes at the repository level, normalized by equivalent uniform infiltration flux applied at the ground surface for two east-west cross-sections and three focusing strategies

In developing its safety case for YM, the DOE is currently conducting a detailed and thorough evaluation of infiltration rates and 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.

3.3 AREA OF CONCERN: DILUTION

3.3.1 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).

3.3.2 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.

3.3.3 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.

3.3.3.1 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 from borehole flow surveys for UE-25b #1 (Lobmeyer, et al., 1983; Lahoud, et al., 1984) and UE-25c #1, #2, and #3 (Geldon, 1993) indicate that the groundwater beneath the proposed site is predominantly moving along thin fracture zones. The localized nature of the flow is apparent from the data presented in Figure 3-4 which is taken from 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 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) fracture zones range from 10^{-1} to 1 m/day [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:

$$DF = \frac{q_{SZ}}{q_{UZ}} \frac{W_{Rep}h}{A_{Rep}} = \frac{q_{SZ}}{q_{UZ}} \frac{4000m \times 10m}{4\times10^5 m^2} = \frac{q_{SZ}}{q_{UZ}} \times 0.1 \qquad (4\text{-}1)$$

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 IPA Phase 2 (Nuclear Regulatory Commission, 1995) for the dry and pluvial conditions, calculated dilution factors range from one to two.

3.3.3.2 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)

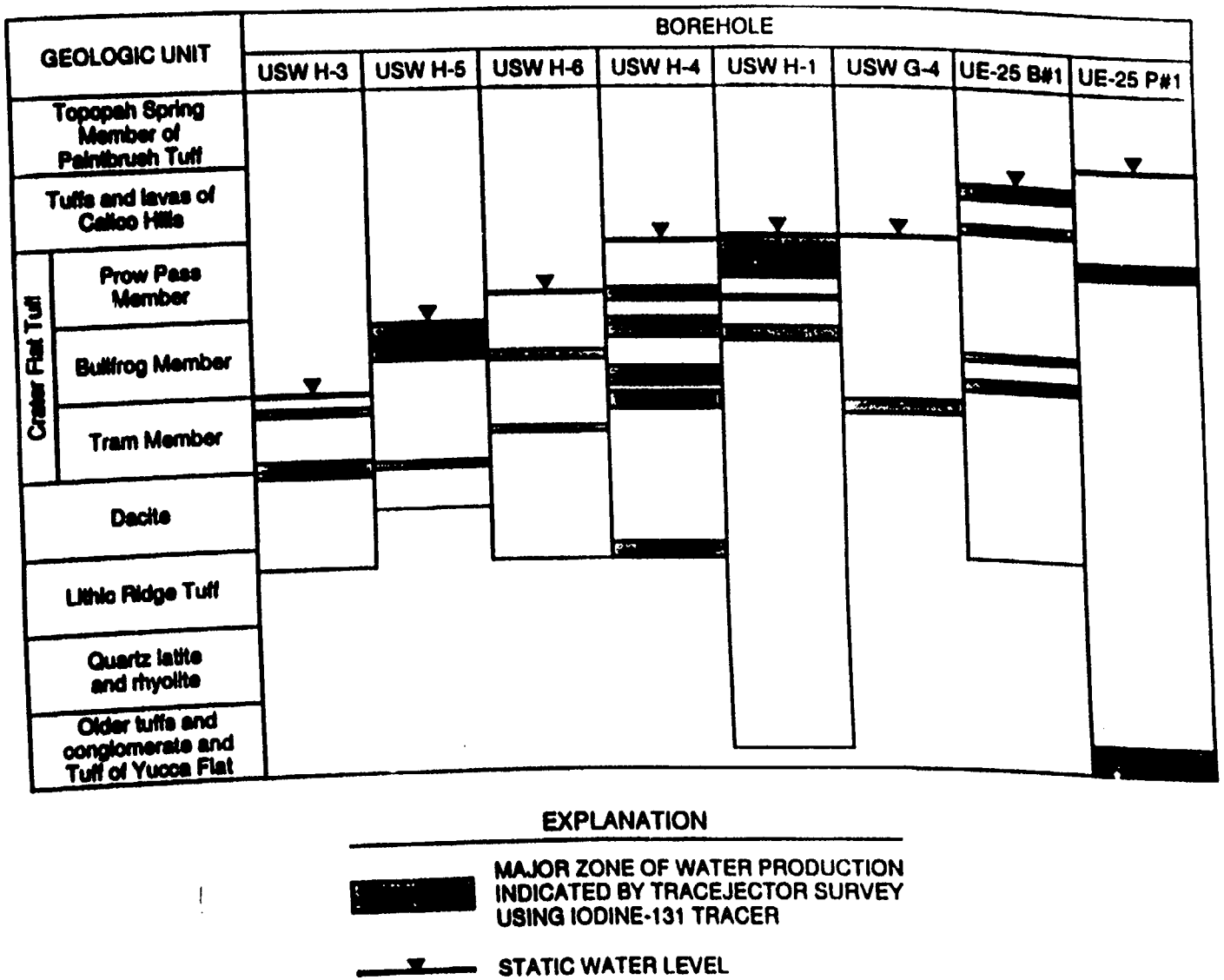

Figure 3-4. Major water-production zones in Tertiary rocks and static water levels in boreholes drilled at Yucca Mountain (taken from Geldon, 1993)

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

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 $\alpha_T / \alpha_L = 1/50$, conservative estimates are $\alpha_T = 10$ m for 5 km and $\alpha_T = 60$ m for 30 km flow paths.

The groundwater flux for the 5 km path length is estimated from available field data as 0.1 m/yr. 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 Czarnecki's (1985) modeling study of 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 3-2. These calculated dilution factors are about 1/3 to 1/5 of those estimated in TSPA-1995.

Table 3-2. 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}

Dilution factors calculated using the maximum q_{UZ} values from the NRC IPA Phase 2 (NRC, 1995) are presented in Table 3-3 and are about 2 to 3 orders of magnitude smaller than those calculated in TSPA-1995. TSPA-1993 (Wilson et al., 1994) present results for a detailed 3-D transport model which indicates dilution factors at 5 km in the range of $5 \leq DF \leq 20$. These estimates are again substantially smaller than those in TSPA-1995.

Table 3-3. 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 groundwater basin (20,000 ac-ft/yr) by the outflow from Jackass Flat/Buckboard Mesa groundwater basin (8,000 ac-ft/yr), which contributes to the total inflow to the Amargosa Desert groundwater basin. It was apparently assumed in TSPA-1995 that the total 20,000 ac-ft of annual inflow to the Amargosa Desert groundwater basin does not already include the 8,000 ac-ft of influent contributed by Jackass Flat/Buckboard Mesa groundwater basin.

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 levels of mixing and dilution that occur in the YM and the groundwater withdrawal areas may be lower than assumed in TSPA-1995.

3.3.4 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 conduct a more 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.

3.4 GENERAL COMMENTS—MATRIX SATURATION

3.4.1 Statement of Concern

The chosen degree of matrix saturation at which fracture flow is initiated is a critical factor in the TSPA calculations, which 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 not adequately conservative.

3.4.2 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 selected "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 that 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 records 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.

3.4.3 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 determining a more realistic and conservative bounding value.

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4 KEY TECHNICAL ISSUE: THERMAL EFFECTS ON FLOW

4.1 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 4-1.

Table 4-1. 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

4.2 AREA OF CONCERN: CALCULATION OF TEMPERATURE AND RELATIVE HUMIDITY

4.2.1 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 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, leading to a temperature increase of about 330 °C (p. 10-26 of Wilson et. al., 1994). In TSPA-1995, the maximum WP temperature is obtained prior to backfilling, with a temperature increase of less than 20 °C (p. 4-24 of TSPA-1995). Another important difference is that a 2D model was used in TSPA-1995 whereas a 3D model was used in TSPA-1993. The 2D model averages 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.

4.2.2 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 4-2. Probably the most significant difference is that TSPA-1993 included a full 3D model of the WP residing in a drift while TSPA-1995 uses a simpler 2D model. The TSPA-1993 results show an increase in WP temperature of about 330 °C (from 190 to 520 °C) after backfill is emplaced, while TSPA-1995 results show negligible effect on WP temperature (ΔT of about 15 °C, an 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.

4.2.3 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 (AML) scenarios. 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, the same processes included in the FEHM code 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.

The thicknesses of each thermohydrologic unit are taken from Figure 4.2-1 of TSPA-1995 while thermal properties are obtained from Table 4.2-3 of TSPA-1995. Some thermal properties are not fully described in TSPA-1995, hence some judgement was exercised. For example, rock wall and WP emissivity values and the method for generation of radiative view factors are not discussed in TSPA-1995, yet must have been addressed based on the last paragraph in Section 4.2.1 of TSPA-1995. Also, the specified properties of the pre-fab support and concrete invert were not found in TSPA-1995. In order to complete the audit review analyses, an effective conductivity model was developed and used for the unbackfilled drift region, and properties for concrete support/invert were assumed.

In an unbackfilled drift with temperatures above 100 °C, thermal radiation will dominate the heat transfer from the WP to the drift wall. The rate of radiative heat transfer is given by (Eq 13.23 of Incropera and DeWitt, 1990):

$$q_{rad} = \frac{\sigma\left(T_{wp}^4 - T_{rw}^4\right)}{\dfrac{1-\epsilon_{wp}}{\epsilon_{wp} A_{wp}} + \dfrac{1}{A_{wp} F_{wp-rw}} + \dfrac{1-\epsilon_{rw}}{\epsilon_{rw} A_{rw}}} \tag{4-1}$$

where

σ = Stefan-Boltzman constant ($=5.67\times10^{-8}$ W m^{-2} K^{-4})

T_{wp} = absolute temperature of waste package surface (K)

Table 4-2. 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

T_{rw} = absolute temperature of rock wall surface (K)

ε_{wp} = thermal emissivity of water package surface (-)

ϵ_{rw} = thermal emissivity of rock wall surface (-)

A_{wp} = area of waste package surface (m^2)

A_{rw} = area of rock wall surface (m^2)

F_{rp-rw} = view factor from waste package to rock wall (-)

In general, the emissivity of rock is large and assumed to be unity in this work. The view factor is F_{rp-rw}=1.0. In addition we use the algebraic relationship:

$$\left(T_A^4 - T_B^4\right) = \left(T_A^2 + T_B^2\right)\left(T_A + T_B\right)\left(T_A - T_B\right) \approx 4\left(T_{avg}\right)^3\left(T_A - T_B\right) \tag{4-2}$$

Equation (4-1) is then reduced to:

$$q_{rad} = A_{wp}\epsilon_{wp}\sigma 4\left(T_{avg}\right)^3\left(T_{wp} - T_{rw}\right) \tag{4-3}$$

The rate of heat transfer in the unbackfilled region using an effective thermal conductivity is given by (Eq.3-27 of Incropera and DeWitt, 1990):

$$q = \frac{2\pi L k_{eff}\left(T_{wp} - T_{rw}\right)}{\ln\left(\frac{D_{rw}}{D_{wp}}\right)} \tag{4-4}$$

where

L = unit depth in third dimension $(=1m)$

k_{eff} = effective thermal conductivity $\left(W\ m^{-1}\ k^{-1}\right)$

Equating Eq. (4-3) and (4-4), and using $A_{wp} = \pi D_{wp} L$, one solves for effective conductivity:

$$k_{eff} = \epsilon_{wp}\left(\frac{D_{wp}}{2}\right)\sigma\ 4\ \left(T_{avg}\right)^3 \ln\left(\frac{T_{wp}}{T_{rw}}\right) \tag{4-5}$$

From Figure 4.2-5 and 4.2-9 of TSPA-1995, the average drift temperature is about 120°C. Assuming ε_{wp}=0.8, D_{wp}=1.8m, D_{rw}=5.0m, one calculates k_{eff}=10 $W\ m^{-1}\ K^{-1}$, which is the value used in our simulation. An effective thermal conductivity approach is also justified and used in TSPA-1993 (Section C.2.3 of Wilson et al., 1994). After backfilling, the value of k_{eff}=0.6 $W\ m^{-1}\ K^{-1}$ was used as specified in Table 4.2-3 of TSPA-1995. The thermal properties of concrete support/invert are not discussed in TSPA-1995 so that they are assumed to be k=1. $W\ m^{-1}\ K^{-1}$, ρ=2,580 $kg\ m^{-3}$, and C=840 $J\ kg^{-1}\ K^{-1}$ (based on Incropera and DeWitt, 1990).

A small portion of the computational mesh near the WP is shown in Figure 4-1 for the 2D simulations using ABAQUS and MULTIFLO. ABAQUS is based on the finite element method so that the geometry is more precise. The MULTIFLO code uses a rectangular grid, so that the WP and drift sizes are based on equivalent cross-sectional areas.

The relative humidity is calculated using the same approach as Eq. 4.2-1 on Page 4-6 of TSPA-1995. The relative humidity 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 vapor pressure at the WP surface is then dictated by the vapor pressure at the drift wall.

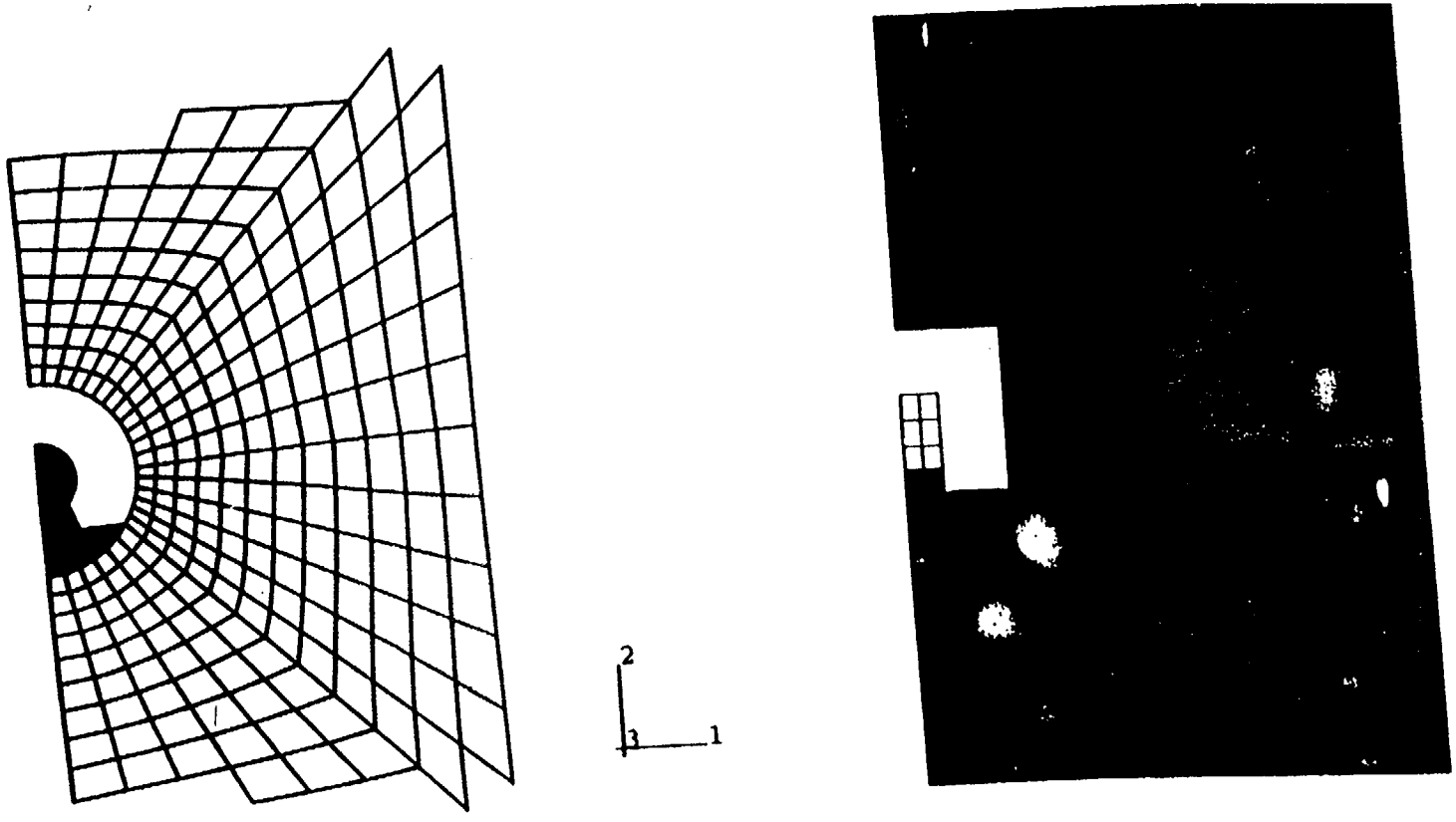

Figure 4-1. Two-dimensional model used by ABAQUS (left) and MULTIFLO (right)

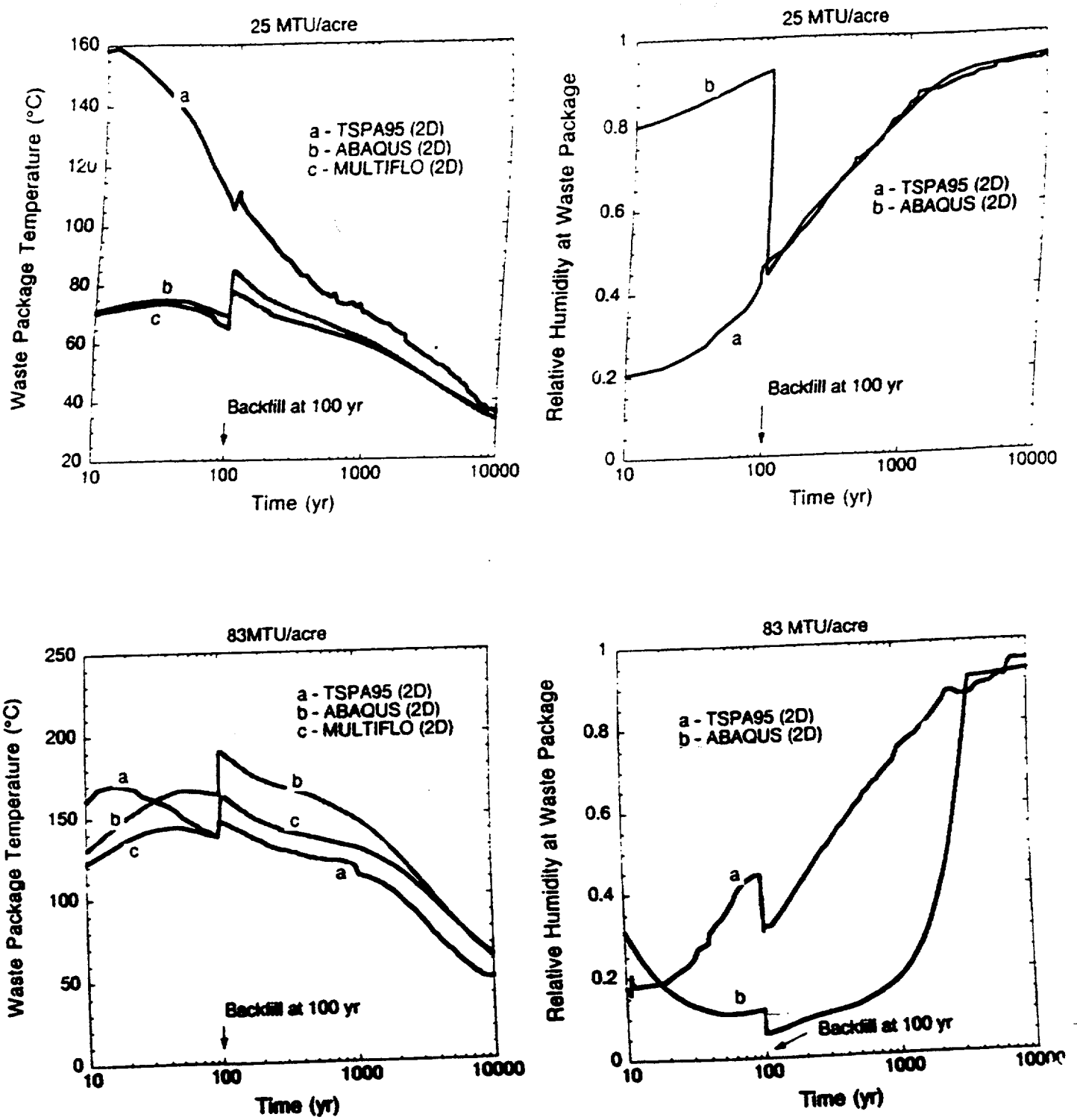

Figure 4-2. Comparison of two-dimensional model results

In Figure 4-2, 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 temperature and relative humidity are in general agreement over longer periods of time (i.e. greater than 100 years). For the first few hundred years, the TSPA-1995 results show a higher WP temperature and resulting lower relative humidity. 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 methodology in TSPA-1995. The report states that a radiative transfer model was employed, but does not discuss how view factors were calculated or how emissivity values for the package or drift wall were obtained.

For the 2D, 83 MTU/acre case, the temperature and relative humidity results are in better agreement. The TSPA-1995 temperatures are essentially the same as the ABAQUS and MULTIFLO code results out to 10,000 yr. The relative humidity is lower for the ABAQUS simulation due to higher waste package temperatures.

The 3D model shown in Figure 4-3 is used to predict WP temperature and is motivated because the 2D model averages the heat source along the drift, resulting in underpredictions of the WP temperature. Calculations were performed to determine the magnitude of the underprediction. In Figure 4-4, 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 near-field thermal evolution of a backfilled WP. The results show that the 3D model predicts higher temperatures throughout the time of interest. The temperature difference is most distinct immediately after backfilling, with a temperature increase of about 40 to 50 °C in both the 25 and 83 MTU/acre cases.

4.2.4 Description of Likely Effects on Performance

Independent calculations conducted by 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, believed to be due to the radiative heat transfer model employed and different assumptions about heat transfer mechanisms. However, the documentation of the model in TSPA-1995 is inadequate to fully explain the differences. 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 predict a significant temperature increase at the time of backfilling. As noted in TSPA-1995, different modeling assumptions can lead to significant differences in results.

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 WP spacing length. This tends to produce lower WP temperatures than those predicted using 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. Rather, it is reported as an unbiased estimate of anticipated conditions. Because the WP thermohydrologic environment is an important factor in the release and transport of radionuclides in the near-field, future TSPAs are encouraged to examine two factors in the calculations: (i) the heat transfer models in the drift prior to backfilling, and (ii) use of 2D versus 3D models.

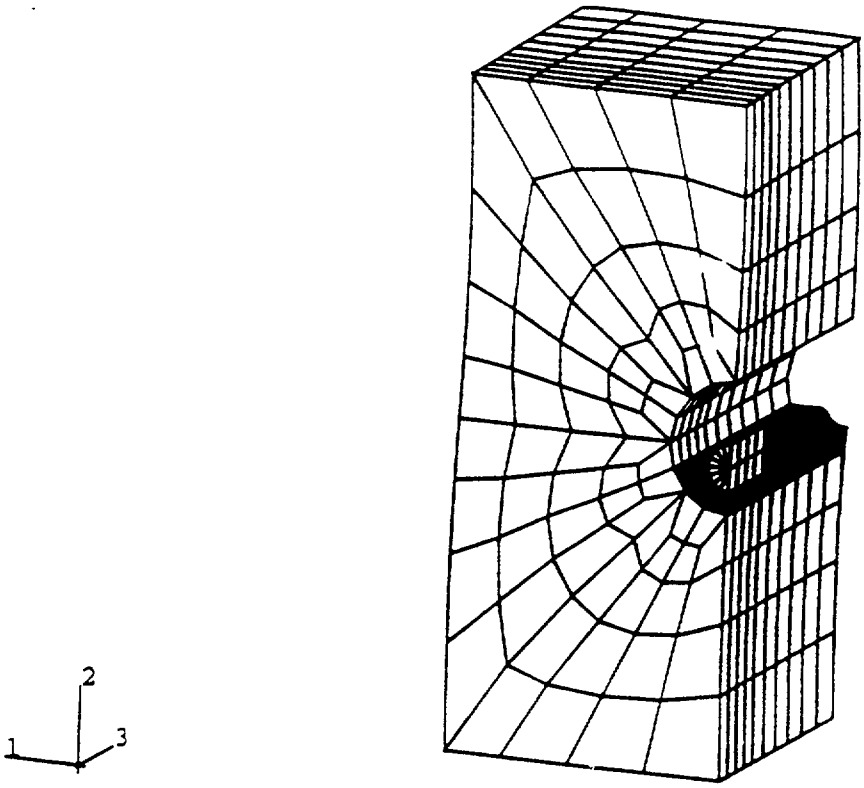

Figure 4-3. Three-dimensional model

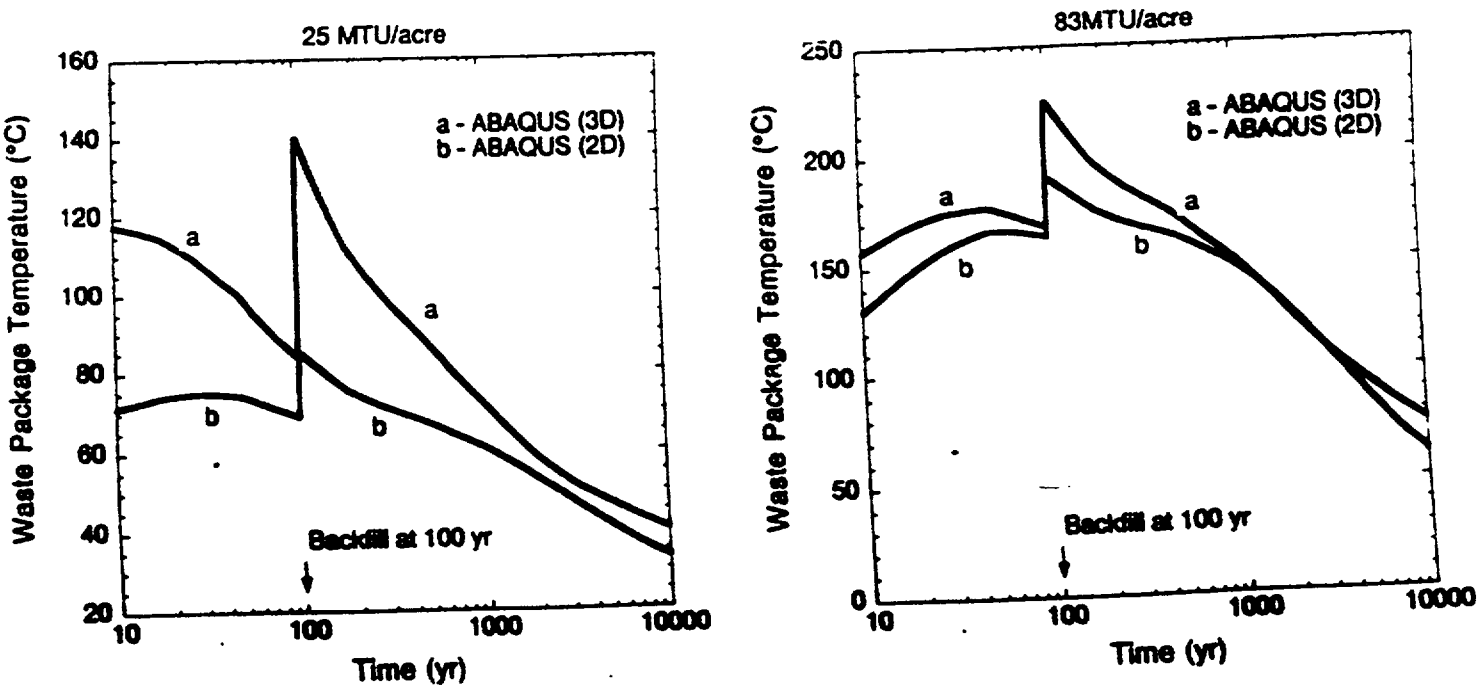

Figure 4-4. Comparison of two- and three-dimensional model results

4.3 GENERAL COMMENTS—THERMOHYDROLOGY

4.3.1 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.

4.3.2 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).

4.3.3 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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5 KEY TECHNICAL ISSUE: CONTAINER LIFE AND SOURCE TERM

5.1 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 5-1.

Table 5-1. 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

5.2 AREA OF CONCERN: WASTE PACKAGE FAILURE MODES

5.2.1 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 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 as relevant modes. 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)

5.2.2 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 DOE WCIS for the YM 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. Humid-air corrosion and general corrosion in the aqueous environment were assumed to be negligible for the inner corrosion-resistant container.

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

$$\ln D_g = a_0 + a_1 \ln t + a_2/RH + a_3/T + a_4[SO_2] \qquad (5\text{-}1)$$

The parameters a_i in Eq. (5-1) 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 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. (5-1) was used for general corrosion of the outer steel container under aqueous conditions

$$\ln D_g = b_0 + b_1 \ln t + b_2/T - b_3 t^{-2} \tag{5-2}$$

The parameters b_i in Eq. (5-2) 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. For pitting corrosion in an aqueous environment the median pit growth rate was expressed as

$$\ln R_p = A - 0.5 \ln t - B/T \tag{5-3}$$

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. (5-1) through (5-3), 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.

5.2.3 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 comprehensively 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 the change in concentration of anionic species in the groundwater resulting from alternate 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. (5-1) for evaluating corrosion of the outer steel barrier may lead to nonconservative estimates of the extent of corrosion. Equation (5-1) 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. (5-2) 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 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. (5-3) 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.

5.2.4 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.

5.3 GENERAL COMMENTS—WASTE PACKAGE BARRIERS

5.3.1 General Comment—Cladding Degradation Modes

5.3.1.1 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.

5.3.1.2 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.

5.3.1.3 Recommendations

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

5.3.2 General Comment—Waste Form Alteration and Radionuclide Release

5.3.2.1 Statement of Concern

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

- Effects of dry oxidation on the surface area and consequent dissolution of spent fuel is inadequately recognized.
- Colloidal release is not included in performance calculations.
- Enhanced release of fission products and gaseous release from fuel are neglected.
- 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.
- 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.

5.3.2.2 Basis for Concern

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.

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, 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.

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.

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.

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.

5.3.2.3 Recommendations

Current Pacific Northwest Laboratories (PNL) (Gray and Wilson, 1995) experimental results should be incorporated in PA. Future Argonne National Laboratory experimental results should be interpreted, modeled and incorporated in PA. (For sample models, see Ahn, 1995b; Manaktala et al., 1995). Future PNL experimental results and some data from reactor operation may be used in PA. 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. 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.

5.3.3 General Comment—Limits of Capillary Barriers

5.3.3.1 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.

5.3.3.2 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 for 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.

5.3.3.3 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 PA's 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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APPENDIX A—DOSE ASSESSMENT CALCULATION

TOTAL SYSTEM PERFORMANCE ISSUE

In addition to Complementary Cumulative Distribution Functions (CCDFs), TSPA-1995 also presented results of calculations based on single values of parameters. One such calculation in TSPA-1995 was the calculation of drinking water dose from ^{237}Np as a function of time based on expected values of infiltration and solubility limits. ^{237}Np was selected for this review because it is very long-lived and an important contributor to dose. Thus the peak ^{237}Np dose occurring at long times will be insensitive to assumptions regarding the thermal period, waste container, and release rates for spent fuel.

DESCRIPTION OF CALCULATIONAL APPROACH

Using expected values reported in TSPA-1995, the dose due to ^{237}Np was calculated by the following procedure:

1) Determine the amount of flow contacting the waste

2) Determine the release rate based on solubility limit

3) Determine contaminant water concentration

4) Determine drinking water dose

5) Compare to TSPA-1995 results

Two calculations were performed, one for the high infiltration rate (1.25 mm/yr), and one for the low infiltration rate (0.03 mm/yr). For the TSPA-1995 audit review calculation, the infiltration rate remained constant (in the TSPA-1995 calculation, the infiltration rate increased). From the TSPA-1995 Figures 7.3-5 to 7.3-8, the fracture drip flux and fraction of packages being contacted by water were estimated. These values were:

Fracture drip flux (low infiltration) = 0.0025 mm/yr
Fracture drip flux (high infiltration) = 0.70 mm/yr
Fraction of packages dripping (low infiltration) = 0.06
Fraction of packages dripping (high infiltration) = 0.50

With a total of 6,468 spent fuel packages (TSPA-1995, page 8–15) the number of packages dripping is 388 for the low infiltration case and 3,234 for the high infiltration case. From these values and the TSPA-1995 capture area per package value of 41 m^2, the amount of water contacting the waste for the low infiltration case is 0.04 m^3/yr and for high infiltration is 92.7 m^3/yr.

Assuming that ^{237}Np will be released at its solubility limit (34 g/m^3 or 0.024 Ci/m^3), releases of 9.6×10^{-4} Ci/yr (low infiltration) and 2.2 Ci/yr (high infiltration) were calculated. The value obtained for the high infiltration case is close enough to the TSPA-1995 maximum annual release rate (2.1 Ci/yr) to verify the assumption of release of ^{237}Np at its solubility limit.

APPENDIX A

DOSE ASSESSMENT CALCULATION

Using the mixing volumetric flow rate of 400,000 m^3/yr (Section 7.6.2) and the ^{237}Np dose conversion factor of 3.2×10^9 mrem/yr (Table 7.6-1), the calculated drinking water doses are 7.5 mrem/yr (low infiltration) and 17,000 mrem/yr (high infiltration).

TECHNICAL FINDINGS

The above dose estimates are approximately 2 orders of magnitude different (higher) than the 1×10^{-4} mrem/yr and 200–300 mrem/yr doses presented in the TSPA-1995 for the low and high infiltration cases, respectively. The apparent extra dilution estimate ' in TSPA-1995 is believed to come from the model abstractions for inter-unit fracture connectivity used in the TSPA-1995 RIP model. Figure 7.4-3 of the TSPA-1995 would seem to indicate that a release could be extended over a much longer period and thus allow for significantly more dilution. For this example, a very short pulse of ^{237}Np is assumed (at a release rate of about 2 Ci/yr, the 70,000 Ci inventory of ^{237}Np in the waste packages would be depleted in less than 35,000 years). However, the TSPA-1995 results (page 9–67) show that ^{237}Np release persists for over a million years. This delayed release is approximately equal to the 2 orders of magnitude increase in dilution necessary for the example results to make sense.

Unfortunately, the parameters used to derive the particle transition rate of random travel length in the fracture is not reported in the TSPA-1995 document, and the extra dilution attributed to the factor is not known. Geochemical information seems to indicate that the fracture water and matrix water have different geochemical properties. The inter-unit fracture connectivity abstraction is a concept that warrants closer inspection in that modifications could reduce potential dose estimates by orders of magnitude.

APPENDIX B

EVALUATION OF MARKOVIAN TRANSPORT MODEL

APPENDIX B—EVALUATION OF MARKOVIAN TRANSPORT MODEL

TOTAL-SYSTEM PERFORMANCE ISSUE

The unsaturated flow transport model used in TSPA-1995, as described in Section 7.4 of the document, was evaluated by comparison to the model used in NRC's IPA Phase 2. Using simplified versions which follow the conceptual models, the similarities and difference between the Markov transition model and the model used in NRC's IPA Phase 2 are evaluated. The TSPA-1995 unsaturated zone transport model uses the Markovian transition model for transport of radionuclides through the geosphere (modeled as four lithologic or hydrostatigraphic layers). The Markovian model is based on the transition of particles (representing radionuclides) through fracture and matrix compartments describing the system.

In the Markov model, particles in both the fracture and the matrix have a velocity in the downward direction through distinct flowtubes. A particle starts in a given pathway (fracture or matrix), with a probability F_{frac} of being in the fracture and $(1-F_{frac})$ of being in the matrix, and moves a distance (Δx), before transitioning to the other pathway (matrix or fracture). The magnitude of the distance moved in a given pathway, Δx, is sampled from an exponential distribution. The time (Δt), required for a particle to move any given dista· ·· is the length of particle movement, Δx, divided by the particle velocity. This velocity takes into account retardation of the particle (particle travel times are longer in the matrix than in the fracture). After each Δt, the particle changes state from fracture to matrix (or vice-versa) and continues moving through the layer(s). If the particle moves past the layer boundary, the travel time is modified for transport to that boundary. Upon leaving a layer, the particle enters the top of the next layer and the process repeats itself until all layers have been transversed. Consequently, the total transition time for a particle to move through the unsaturated zone is the sum of the travel times (Δt) for each layer.

DESCRIPTION OF CALCULATIONAL APPROACH

IPA Phase 2 employed NEFTRAN, a one-dimensional network model. An approximation of this approach was used for comparison to the DOE TSPA-1995 approach described above. Like the Markov model, the NEFTRAN one-dimensional algorithm starts with a particle either in the matrix or fracture state, with a probability F_{frac} of being in the fracture and $(1-F_{frac})$ of being in the matrix. The particle then moves entirely through a given layer in that state. At the top of the next layer the particle again is either in the fracture or the matrix, with probabilities again F_{frac} and $(1-F_{frac})$, respectively. Since there is no change of state for the particle except at the top of each layer, it is not necessary to actually sample probabilities for each particle. For a four layered model there can only be 2^4 (16) possible pathways with the travel time and probability uniquely known for each pathway. This algorithm description differs from NEFTRAN in that it ignores longitudinal dispersion. However, this should not have a large effect on the outcome, as dispersion was shown to have only a minor effect on results in the IPA Phase 2 analysis.

Comparison of the two models (see Figure B-1) was conducted with a 5,000 particle trial on a single column like that used in the TSPA-1995 (4 layers in the unsaturated zone using data typical of the high infiltration case, 2 mm/yr). Matrix and fracture particle velocities, F_{frac}, and layer thickness values used in comparison trial calculations were taken from TSPA-1995. The retardation factor in the fractures was taken as unity (no retardation). The retardation factor for the matrix is a representative value estimated from the information of K_d and density given in the TSPA-1995.

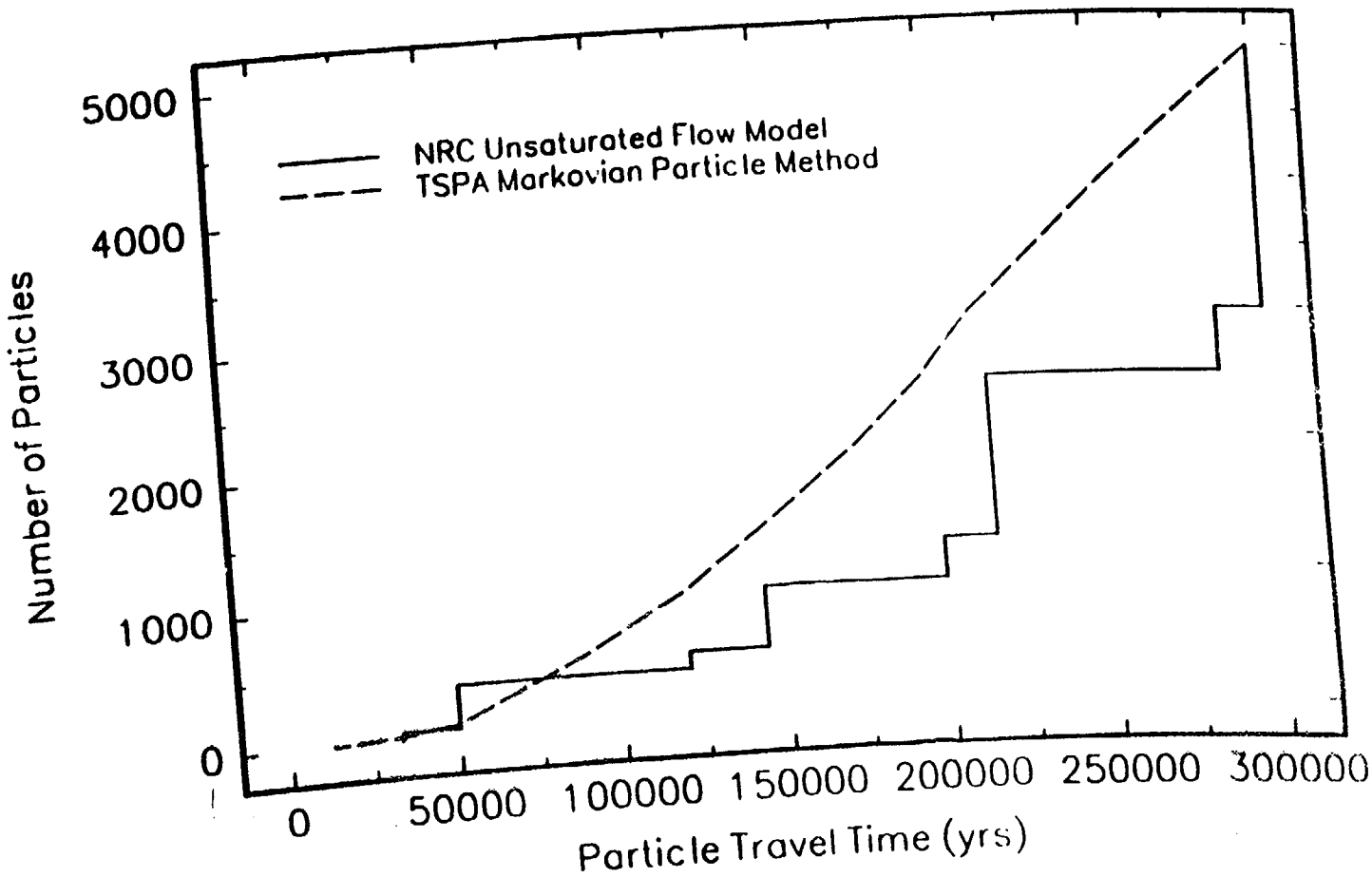

Figure B-1. Comparison of particle travel times for RIP Markov model and TPA NEFTRAN code

Results of this trial apply only to an instantaneous pulse release to a single column in the unsaturated zone. The comprehensive scenario differs in a number of important respects:

1. There would be multiple columns with different layer thicknesses that would also include the transport through the saturated zone to the points of use.

2. The release rates to the top of the column would be continuous rather than an instantaneous peak.

3. The release rates and velocity vary in time from column to column.

TECHNICAL FINDINGS

Results of an instantaneous release 5,000 particle trial for each model have obvious differences. The particle arrival times are much more spread-out using the TSPA-1995 Markov model. This is expected, as the pathways and particle travel times are much more random in character compared to the limited number of pathways specified in the IPA Phase 2 model. The NRC model would lead to a higher peak concentration at an earlier time than would the Markov model. The Markov model also disperses the pulse over a much longer time.

The attached plot presents a CDF for the fastest 1,000 out of 5,000 particles for one realization of each model using the same hydrologic parameters. It shows that the IPA Phase 2 model has a significantly greater number of particles at about 35,000 to 50,000 years. The absolute values of the travel times is not significant because they are dependent on the hydrologic parameters of the realization, however, the comparison of the models is significant.

The TSPA-1995 value chosen for the parameter λ appears reasonable at first glance: "For TSPA-1995, the default particle-transition rate for the Markovian dispersion process between fracture and matrix is set equal to the inverse of the pathway length. This means that on average a radionuclide particle will travel the length of the pathway (e.g., through the TSw) within a fracture, before transitioning to the matrix-flow mode or vice-versa." This overstates the conservativeness of the model used for the following reasons:

1. The transition distance (Δx) sampled from the exponential distribution is weighted toward values much less than the layer thickness (L). The area under the curve of the exponential distribution between $\Delta x = 0$ and 1 is $\int e^{-x} dx = 1 - e^{-1} = 0.63$. Over 63 percent of the particles transition to the matrix, with its much slower travel times, before reaching the end of the layer. Similarly, over 39 percent would have transitioned before reaching L/2 and over 18 percent would have transitioned before reaching L/5. This constitutes a considerable amount of credit attributed to the desirable properties of the matrix.

2. There is no field evidence of any significant matrix diffusion at this site, and some evidence to the contrary (e.g., isotopes in perched water bodies are significantly out of equilibrium with the rock in which they are in contact).

In conclusion the Markov transition model employed for the radionuclide transport calculations in TSPA-1995 appears to give too much credit for flow and transport in the matrix. There is practically no justification for the choice of this model or its parameters. The results of the model lead to the conclusion of a substantially lower peak concentration, spread over a much longer time than would be derived using a more conservative transport model. The model used in the next TSPA should account for the interchange between matrix and fracture by molecular diffusion but should have more defensible parameters. The Markov transition model or something similar may be applicable for the performance assessment calculations if it can be defended by more complete models.