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REVIEW OF THE UNSATURATED ZONE MODELS USED TO SUPPORT THE VIABILITY ASSESSMENT OF A REPOSITORY AT YUCCA MOUNTAIN

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ABSTRACT

The purpose of this report is to provide an independent technical review of the various unsaturated zone (UZ) flow and radionuclide transport (RT) models used in the Viability Assessment of a Repository at Yucca Mountain, recently issued by the U.S. Department of Energy (DOE). The focus of the review is on the appropriateness and applicability of the key assumptions and conceptualizations that underlie the DOE approaches to UZ flow and RT modeling and predictions of repository performance. Particular attention is given to those assumptions and conceptual models shown in both the Nuclear Regulatory Commission (NRC) and the DOE performance assessment calculations to have a potentially significant impact on the proposed high-level waste repository performance. There are four areas of review covered in this report: DOE site-scale UZ flow model, infiltration and flow above the repository, distribution of flow into drifts at the repository horizon, and UZ flow and RT from the repository to the water table. Summaries of technical concerns and proposed paths to resolution are provided for each review area.

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QUALITY OF DATA AND CODE DEVELOPMENT

DATA: There are no original CNWRA-generated data contained in this report. All Data used to support conclusions in this report are taken from documents published by U.S. Department of Energy (DOE) contractors and supporting organizations who operate under the quality assurance (QA) program developed for the Yucca Mountain Project. The reader should refer to data source documents, referenced throughout this report, to determine data QA status.

CODE: Modeling to determine drift seepage percolation thresholds, described in section 4 of this report, was performed using CNWRA-developed MULTIFLO code, Version 1.2β, which has been developed following the procedures described in the CNWRA Technical Operating Procedure, TOP-018, which implements the guidance contained in the CNWRA QA Manual.

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1 INTRODUCTION

The purpose of this report is to provide an independent technical review of the various unsaturated zone (UZ) flow and transport models used in the viability assessment (VA) of a repository at Yucca Mountain (YM), recently issued by the U.S. Department of Energy (DOE, 1998). The VA includes a total system performance assessment (TSPA), hereafter referred to as the TSPA-VA, of the proposed YM high-level nuclear waste (HLW) repository. The key documents that describe the most recent methods and models used to support the TSPA-VA sections dealing with the UZ are listed in table 1-1.

The DOE documents listed in table 1-1 provide generally well-written and succinct descriptions of their respective modeling efforts and TSPA abstraction methods. In this report we do not attempt to repeat the model and abstraction descriptions already proffered so articulately by the DOE and its contractors. Rather, we focus on the appropriateness and applicability of the key modeling assumptions and conceptual models that underlie the DOE approaches to modeling UZ flow, radionuclide transport (RT), and repository performance. Particular attention is given to those assumptions and conceptual models shown in both the U.S. Nuclear Regulatory Commission (NRC) and the DOE performance assessment (PA) calculations to have a potentially significant impact on the proposed HLW repository performance. To this end, a technical review of the supporting documents listed in table 1-1 is performed with respect to the following aspects of the flow system.

- Site-scale UZ model;
- Infiltration and deep percolation from the surface to the repository horizon;
- Percolation flux at the repository horizon and seepage into drifts; and
- Flow pathways and RT from the repository to the water table.

The task of characterizing the proposed HLW repository at YM to a level sufficient for licensing is a challenge that DOE and its contractors continue to make great efforts to meet. Most, if not all, of the technical concerns, data gaps, and conceptual model limitations raised throughout this report have already been acknowledged by, or brought to the attention of, DOE researchers at various technical exchanges and workshops during the development of the TSPA-VA. Several ongoing research efforts may ultimately result in resolution of many of the issues raised in this report. Three such efforts are: (i) tracer injection tests at Busted Butte, (ii) the large-scale heater test in the Exploratory Studies Facility (ESF), and (iii) the infiltration and seepage studies at Alcove 1 of the ESF.

In addition to the technical review of the DOE approach used in the TSPA-VA, each of the chapters of this report also contains

- A summary of potential alternate conceptual models;
- A summary of technical concerns regarding the DOE modeling approaches, supporting site characterization data and TSPA abstraction methods; and
- Suggested paths to resolution of technical concerns.

Readers primarily interested in outstanding technical concerns and paths to resolution may wish to proceed directly to those sections and refer to the more technical discussions of DOE approaches and alternate conceptual models as necessary.

Table 1-1. Areas of review and key supporting documents reviewed in this report

Review Topic	Key Supporting Documents
Site-Scale Unsaturated Zone Flow Model of Yucca Mountain	Bodvarsson et al., 1997; Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (chapter 2); U.S. Department of Energy, 1998 (volumes 1 and 3)
Site-Scale Unsaturated Zone Radionuclide Transport	Robinson et al., 1997; Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (chapter 7); U.S. Department of Energy, 1998 (volumes 1 and 3)
Drift Seepage and Capillary Diversion Models	Civilian Radioactive Waste Management, Management & Operating Contractor, 1998 (chapter 2); U.S. Department of Energy, 1998 (volumes 1 and 3)
Total System Performance Assessment Abstraction for the Viability Assessment	Civilian Radioactive Waste Management, Management & Operating Contractor, 1998 (chapter 2); U.S. Department of Energy, 1998 (volume 3)

2 SITE-SCALE UNSATURATED ZONE FLOW MODEL

Researchers at the Lawrence Berkeley National Laboratory (LBNL) have developed a 3-dimensional (3D), dual-permeability, site-scale UZ flow model of YM to predict flow pathways from the YM ground surface to the regional water table (Bodvarsson et al., 1997). This model (hereafter referred to as the LBNL UZ Flow Model) explicitly considers subsurface flow of air and water in and between fracture and matrix by modeling them as two interacting continua. This type of model is referred to as a dual-permeability model (DKM). The model incorporates many of the large-scale geologic features found in the UZ at YM, including stratigraphy, faults and associated offsets, dipping beds, and zones of geochemical alteration.

The applicability of several key assumptions in the LBNL UZ Flow Model is addressed throughout this report. These assumptions include

- The DKM adequately represents fracture-matrix flow and interaction.
- Steady-state infiltration is an adequate approximation of natural conditions.
- The range of laboratory-measured matrix hydraulic parameters is representative of *in situ* matrix conditions.
- Fracture hydraulic properties can be derived from air permeabilities, fracture frequencies, and fracture orientations measured in drill holes and in the ESF.
- The van Genuchten/Mualem functional form, used to determine fluid pressure and relative permeability as a function of saturation, is satisfactory to represent the saturation and desaturation behavior of both matrix and fractures.
- The fracture-matrix (F/M) connection area is reduced below the geometric area implied by fracture spacings used. Physically, this reduction represents effects of channelization of flow in fractures.
- Heterogeneity within a unit is not important (i.e., hydrogeologic units are homogenous).
- The water table elevation remains fixed for any given climate scenario.

As currently conceptualized in the LBNL UZ Flow Model, the downward flow of infiltrating water occurs in both fractures and rock matrix. It is generally agreed that, of the two flow domains, water flowing in rock matrix is far less likely to drip onto a waste package (WP), owing to the relatively strong capillary attraction. In addition, RT through rock matrix is slow and subject to significant sorption on mineral surfaces. Thus, the distribution of infiltrating water fluxes between fractures and rock matrix directly affects the volume of water that may eventually contact WPs. These two factors have been shown in both RT times and DOE and NRC sensitivity analyses to significantly affect RT times and peak radiation doses [e.g., U.S. Department of Energy, 1998 (volume 3, section 5.1); Nuclear Regulatory Commission, 1999]. Because TSPA predictions of repository performance depend on F/M flux distributions (also referred to as flow fields), it is important that TSPA analyses consider a set of possible flow fields that bound the uncertainty in UZ fracture and rock matrix hydraulic properties.

2.1 REVIEW OF U.S. DEPARTMENT OF ENERGY APPROACH TO TOTAL SYSTEM PERFORMANCE ASSESSMENT FOR THE VIABILITY ASSESSMENT

The LBNL UZ Flow Model has two important end uses in the DOE TSPA-VA analyses: (i) to determine the distribution of water percolation fluxes reaching the repository horizon and (ii) to provide groundwater flow velocity vectors at each 3D model element beneath the repository for use in the Unsaturated Zone Radionuclide Transport Model (Robinson et al., 1997). Incorporation of this flow model into the TSPA-VA base case is accomplished using three hydrologic property sets to encompass the range of uncertainty in the conditions likely to exist. These three property sets are calibrated using three sets of assumptions [U.S. Department of Energy, 1998 (volume 3)]: (i) the base infiltration case (infiltration = I) with mean (estimated) fracture alpha (α_f) value,[1] which represents the DOE best estimate of current infiltration conditions; (ii) a case with infiltration equal to *I*3* and maximum α_f, which represents a pessimistic (very wet) estimate for current infiltration; and (iii) and a case with infiltration equal to *I/3* and minimum α_f, which is deemed to represent the most optimistic (very dry) estimate of current infiltration.

There were originally five calibrated base case property sets in the TSPA-VA: the three just mentioned, plus a *I*3* case with minimum α_f and a *I/3* case with maximum α_f. These latter two were dropped from the TSPA-VA base case because they were found to be similar to the other *I*3* and *I/3* cases with different α_f values. In other words, the TSPA-VA model results were not sensitive to the assumed value of α_f. Conversely, the LBNL UZ Flow Model calibration was shown to be very sensitive to α_f. [(Bodvarsson et al., 1997, (chapter 6)]. In light of the flow model sensitivity to α_f the authors are concerned by the fact that the TSPA-VA model results show little sensitivity to this important parameter. As discussed in section 2.1.2 of this report, this lack of TSPA sensitivity to α_f is apparently an artifact of the UZ flow model calibration process.

In addition to the three base case property sets, the TSPA-VA also contains a sensitivity analysis using an alternate conceptual model of UZ flow, referred to as the DKM/Weeps model. The DKM/Weeps model has a significantly reduced F/M reduction factor to induce more fracture flow. This DKM/Weeps model bears no resemblance to the Weeps model used in previous TSPA efforts (e.g., Wilson et al., 1994). The earlier Weeps conceptual model postulated locally saturated zones, or weeps, that contacted the repository at discrete locations, whereas the TSPA-VA DKM/Weeps model simply uses a F/M reduction factor equal to the upstream fracture relative permeability.

In this section, the matrix and fracture properties assigned to the property sets used in the TSPA-VA are examined. To this end, the following subsections contain reviews of (i) the matrix and fracture hydraulic property characterizations used to constrain the UZ flow model calibration, (ii) the model calibration process, and (iii) the parameter sets used in the TSPA-VA analyses.

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[1]The van Genuchten alpha parameter is one of the several parameters used by van Genuchten (1980) to describe the relationship between the saturation of a porous medium and the fluid capillary pressure—also referred to as moisture retention characteristics. This parameter is often assumed to equal the inverse of the air-entry pressure (i.e. the pressure required to force air into a saturated porous medium or force water out.)

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2.1.1 Matrix and Fracture Hydraulic Properties

Calibrated matrix and fracture hydraulic properties are assumed homogenous within each model layer throughout the entire site-scale model. This assumption of intra-layer homogeneity precludes consideration of discrete fast flow paths through the UZ, except where vertical fault zones are incorporated into the model.

Matrix Properties

The hydraulic properties assigned to represent rock matrix in the LBNL UZ Flow Model are based on numerous core sample laboratory measurements reported by Flint (1998). These measurements include matrix permeability and moisture retention characteristics. The moisture retention characteristics are expressed using the van Genuchten (1980) parameters α_m and m_m to define the constitutive relationship between matrix saturation and fluid capillary pressure. The most important van Genuchten parameter for model calibration is the alpha (α) parameter, which is inversely related to the capillary pressure at which air can just begin to enter a saturated porous medium.

The geometric mean of the laboratory permeability measurements for each layer type was used as the initial guess for model calibration. Data from samples with permeability below measurement limits were excluded from determination of the geometric mean, which resulted in a slight bias toward higher matrix permeability for some layers. During calibration, the matrix permeability was constrained according to the standard deviations given by Bodvarsson et al. [1997 (table 6.2.7-1)].

Despite the wealth of laboratory and field data from which to characterize rock matrix properties, considerable uncertainties still exist. For example, methods for measuring matrix saturations may be biased if dryout is induced by sample collection methods, or if slight sample expansion occurs upon release from *in situ* stresses. The uncertainty in rock matrix hydraulic properties is also supported by a modeling study (Winterle and Stothoff, 1997) that showed use of laboratory-measured hydraulic properties results in modeled water imbibition rates considerably higher than rates observed in the laboratory sorptivity tests (Flint et al., 1996). Additionally, preliminary measurements in the East-West Cross Drift at YM indicate that matric potentials (capillary pressures) are higher than predicted based on observed matrix saturations and laboratory-measured hydraulic properties. These uncertainties regarding *in situ* rock matrix saturations and laboratory-measured hydraulic properties all indicate that the fraction of flow in rock fractures may be significantly greater than is presently considered in TSPA-VA analyses, especially in areas where percolation fluxes are low.

Fracture Properties

Fracture hydraulic properties used in the LBNL UZ Flow Model include permeability and the van Genuchten (1980) moisture retention parameters, α_f and m_f. Initial estimates and model calibration constraints for these parameters are based on fracture frequency data and on air permeability testing. For the TSPA-VA analyses, the base case fracture permeability is obtained by calibrating one-dimensional (1D) UZ stratigraphic column models to match observed borehole saturation profiles and borehole gas pressure responses to barometric pressure changes [Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (chapter 2)]. Calculated minimum, mean, and maximum values for α_f are used to obtain the three calibrated UZ flow fields sampled in the TSPA-VA base case analysis [U.S. Department of Energy, 1998 (volume 3)]. A best-guess value for m_f is assigned for each model layer in all of the calibrated flow fields used in the TSPA-VA analyses, with the constraint that m_f must be equal to or greater than the matrix m value [Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (chapter 2)]. Initial estimates of fracture permeability are obtained from borehole air permeability measurements.

Use of the van Genuchten (1980) moisture retention parameters (α_f and m_f) tacitly implies that fractures are viewed as porous media with a continuous range of pore sizes. The assumed variations in fracture apertures between fractures and within each fracture provide the basis for using a fracture continuum model. Similar to the bundle of tubes model for porous materials, the distribution of aperture sizes in a fracture system controls water retention and saturation-dependent relative permeability. In theory, the value assigned to the α_f parameter in any model grid block should be related to the largest aperture sizes encountered on a grid-block scale; the value assigned to m_f is related to the range and distribution of aperture sizes from narrowest to widest. However, little is known about the distribution of fracture apertures, as the ESF fracture survey measurements predominantly include only the larger apertures. A more detailed study of fracture aperture distributions over a range of sizes may prove useful for reducing uncertainty in appropriate values for fracture moisture retention parameters. For example, if it could be shown that fracture apertures follow a power-law distribution, extrapolation of aperture sizes could be used to develop moisture retention characteristics or estimate permeability.

The values assigned to m_f for TSPA-VA analyses remain unchanged for all of the TSPA-VA UZ parameter sets. Reasonable ranges for α_f used in TSPA-VA analyses are estimated from calculated effective fracture apertures [Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (chapter 2)]. Minimum, mean, and maximum values for α_f are calculated based on (i) a range of borehole air permeability estimates; (ii) mean fracture frequencies, estimated from boreholes, and ESF line surveys; (iii) the assumed validity of the cubic-law, which treats permeability as proportional to the cubed fracture aperture; and (iv) the assumption that α_f is equal to the inverse of capillary rise, calculated from the Young-Laplace equation for planar fractures. The fracture frequency estimates primarily rely on the detailed line survey of the ESF; borehole survey data is also used for units not present in the ESF. For the nonwelded units of the Calico Hills Formation, fracture frequency data from the PTn are used as an analog.

The TSPA-VA approach to bounding the reasonable range for α_f could be improved in two ways. First, the value assigned to α_f should be based on the largest aperture sizes, not on the mean or effective size. Using the largest fracture apertures as a basis for estimating α_f would result in higher values; this would result in less capillary suction in the fracture continuum, and thereby, in lower fracture saturation. Second, the ESF fracture frequency data used to estimate α_f should be corrected to account for the under-representation of fractures that intersect the ESF at low angles. Figure 2-1 illustrates a rather dramatic difference in the characterization of fracture data from a 500-m section of the ESF—between stations 30+00 and 35+00—after applying the Terzaghi (1965) correction method. It can be seen that correction results in an increase in the estimated fracture frequency from 4 m^{-1} to 6.6 m^{-1}. Increased fracture frequency would result in calculation of lower effective fracture apertures and hence, lower values of α_f. Lower values of α_f result in predictions of greater fracture saturations. Although these two shortcomings in estimation of α_f tend to have offsetting effects on predicted fracture saturations, it is not clear if either would have a dominant effect. Therefore, increased confidence in estimates of α_f could be gained by adopting these two improvements.

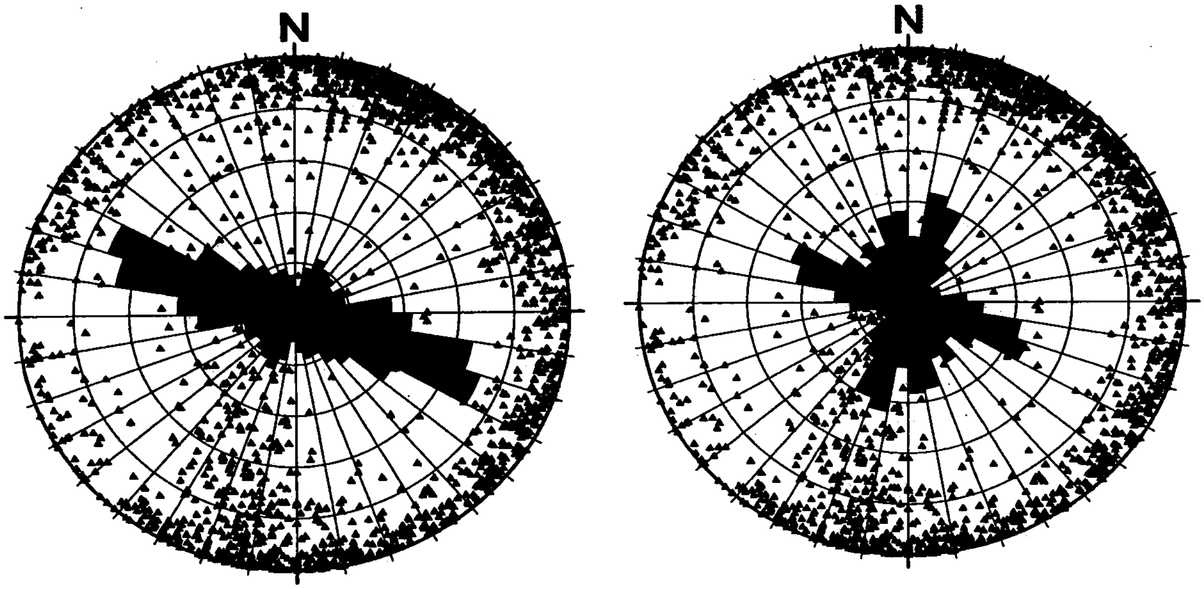

Figure 2-1. Comparison of fracture frequency and orientation data before (left) and after (right) applying the Terzaghi (1965) correction. Applying the correction has two important consequences: (i) the mean fracture frequency over the interval increases from 4 m^{-1} to 6.6 m^{-1} and (ii) the WNW-trending fracture set no longer dominates the distribution as NNE- and NNW- trending fracture sets become evident.

2.1.2 Lawrence Berkeley National Laboratory Unsaturated Zone Flow Model Calibration

The LBNL UZ Flow Model calibrations were performed by simultaneous inversion of a number of 1D submodels, each associated with a borehole. Problems with 1D flow model calibrations arise for areas below the repository horizon where the combined matrix and fracture permeability is less than the mean infiltration rate. Under such conditions, 1D flow models predict the formation of perched water and fail to account for lateral diversion around low-permeability zones. As such, the next calibration of the LBNL UZ Flow Model will be a 3D inversion as shown in Civilian Radioactive Waste Management System, Management & Operating Contractor (1998) and also discussed in the TSPA UZ Abstraction Workshop, December 13–16, 1998. The 3D inversion will better account for lateral flow below the repository, a topic important for transport calculations.

For each 1D calibration, there are approximately 150 parameters in the flow model that must be estimated to achieve an optimal match to the 300 rock matrix saturation measurements. The approach used to develop TSPA-VA parameter sets was to honor the more reliable matrix property data to the extent possible, while varying the less certain fracture parameters for model calibration. To this end, Bodvarsson et al. (1997) obtained a calibrated best-fit set of model parameters by assuming the present-day infiltration rate (I) and allowing rock matrix permeability to vary in addition to the fracture parameters. The matrix permeability was constrained to plus or minus a log-transformed standard deviation from the geometric mean: for many of the model layers, this allowed for significant increases in matrix permeability to match observed matrix saturations.

From review of the parameter sets used to develop the three TSPA-VA base case flow fields [Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (tables 2-19 through 2-23)], it appears that all rock matrix properties and fracture permeabilities from the Bodvarsson et al. (1997) best-fit calibration are held at fixed values for the all of the UZ flow model calibrations. The calibrated parameter sets considered for the TSPA-VA represents three assumed infiltration rates (*I*3*, I, and*I/3*) and three assumed α_f values (minimum, mean, and maximum).

For each of the five UZ flow model base case calibrations, the infiltration rate and fracture and matrix hydraulic properties all appear held constant. This leaves only a single model calibration parameter—the F/M interface reduction factor—used to slow the modeled rate of mass transfer between fracture and matrix continua. Conceptually, the physical basis for an F/M reduction factor lies in the fact that relatively few fractures are thought to actively flow under ambient conditions, and the water in these few fractures is likely to be channelized, resulting in a reduced F/M interface area. Unfortunately, there is presently no available characterization method to determine an appropriate value for this parameter. Thus, the F/M reduction term is treated as an unconstrained UZ model calibration parameter. Concerns with the parameter sets that result from this single-parameter calibration approach are discussed in section 2.1.3.

For calibration of the TSPA-VA base case flow fields, the F/M reduction factor is assumed constant for each model layer. A problem with using layer-specific constants for the F/M reduction factor is that the factors are likely saturation-dependent. This fact is recognized by DOE, and the effect of this saturation dependence is investigated in an alternate conceptual model referred to as the DKM/Weeps model [Civilian Radioactive Waste Management System, Management & Operating Contractor,1998 (chapter 2)], in which the F/M reduction factor is set equal to the saturation-dependent upstream fracture relative permeability. Because the value of the F/M reduction factor is obtained deterministically in the DKM/Weeps model, it was necessary to introduce a new calibration parameter—a scaling factor used to globally increase or reduce the relative permeability value assigned to the F/M reduction factor [Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (chapter 2, section 2.6.1.2)].

Liu et al. (1998) present a framework for estimating the F/M reduction term by including it in UZ constitutive relationships and accounting for active fractures as a portion of all fractures. The three components of this type of F/M reduction factor are (i) interface area of active fractures relative to the interface area of all fractures with the matrix, (ii) the number of active fractures relative to all of the fractures, and (iii) active fracture spacing relative to spacing pertinent for all fractures. Each component is approximated by the value of fracture saturation raised to the power of an exponent. This exponent, which can vary from 0 to 1, becomes the calibration parameter rather than the F/M reduction term. DOE is considering the incorporation of this active fracture model into the LBNL UZ Flow Model (based on discussions at the TSPA UZ Abstraction Workshop, December 13–16, 1998, in Albuquerque, New Mexico).

2.1.3 Parameter Sets Used in the Total System Performance Assessment for the Viability Assessment

Because parameter uncertainty in the LBNL UZ Flow Model cannot be completely eliminated, the parameter sets used to obtain UZ flow fields for TSPA analyses should reasonably bound the range of possible outcomes for repository performance predictions. The parameter sets used in TSPA-VA include the previously described three base case model realizations and the DKM/Weeps alternative model realization. All the UZ flow fields obtained from these parameter sets result in modeled mass fluxes from the repository to the water table significantly slowed by flow through low-permeability rock matrix. For example, in DOE sensitivity analyses for the long-term average (LTA) climate scenario, the bimodal distribution of conservative solute arrival times show more than 70 percent of mass flux is slowed en route to the water table by matrix flow, while the remainder arrives via fast fracture pathways [U.S. Department of Energy, 1998 (volume 3, figure 3-11)].

The authors are concerned that the variety of UZ parameter sets used for TSPA-VA analyses does not adequately reflect the present level of parameter uncertainty. This concern stems from the fact that, during calibration of the TSPA-VA parameter sets, matrix properties were held constant and models were calibrated to match observed matrix saturations. An artifact of this approach is that the calibrated UZ flow fields at any given infiltration rate are largely independent of the assumed fracture continuum properties. This occurs because the parameter sets using minimum, mean, and maximum α_f values are calibrated by adjusting the F/M reduction factor to offset any resultant changes in mass transfer rates between fractures and matrix. For example, a higher α_f value can result in a larger hydraulic gradient driving water across the F/M interface; this effect is offset by using a smaller F/M reduction factor to limit F/M mass transfer. The result is that the distribution of flow between fractures and matrix remains effectively the same. Even in the alternative DKM/Weeps model scenarios, an additional calibration parameter is used to force matrix saturations to match observed values more closely. As a result of this calibration approach, the UZ flow fields used in the TSPA-VA do not reasonably bound the uncertainty in either rock matrix or fracture hydraulic properties.

An additional concern is that volume-averaging over large grid blocks and the assumption of homogenous layer properties preclude consideration of heterogeneity-induced bypassing of nonwelded tuff layers; thus, the base case results may be overly optimistic. Volume averaging for site-scale flow modeling does not allow the details necessary to define likely transport paths or to conduct drift-scale modeling. The objectives of a transport model may be more adequately addressed by the incorporation of heterogeneity in a smaller-scale model. Similarly, the objectives of determining the distribution of seepage into drifts may be more adequately addressed by the incorporation of heterogeneity into an alternative approach, such as a discrete fracture or Weeps model. As pointed out by Preuss et al. (1997), no single model can address all objectives, especially when spatial and temporal averaging scales change.

Finally, the UZ flow fields obtained from model calibrations are not consistent with the observed presence of bomb-pulse ^{36}Cl at repository depths (e.g., Fabryka-Martin, et al., 1997) and perched water geochemical evidence that indicates rapid bypassing of the PTn layer [(Bodvarsson et al., 1997 (chapter 15); NRC, 1998 (section 4.4.2.5)]. While large calibrated values of the F/M reduction factor for the PTn may be consistent with the UZ conceptual model of predominantly matrix flow in this unit, the resulting travel times in excess of a thousand years to the top of the tsw31 unit fail to explain the ^{36}Cl observations and perched water geochemistry. A change in the interaction factor for the PTn sufficient to explain these observations may be well within the range of parameter uncertainty. Alternate conceptual models for fast UZ flow paths are discussed in section 3.2 of this report.

2.2 SUMMARY OF CONCERNS

A summary of concerns includes

- The 1D inversions of the site-scale model do not adequately represent the impact of lateral flow, resulting in higher calibrated values of matrix permeability in the nonwelded layers below the repository horizon.

- The values assigned to fracture continuum hydraulic properties, α_f and m_f, in the TSPA-VA parameter sets are not justified by the distribution of fracture apertures observed on the model-grid scale. Additionally, the calculated range of α_f values considered in the TSPA-VA analyses may be biased because ESF line surveys of fracture frequency have not been corrected to account for the underrepresentation of fractures that intersect the ESF at low angles. Underestimation of fracture frequency results in overestimation of effective fracture apertures which, in turn, results in overestimation of α_f.

- The parameter values assigned to rock matrix hydraulic properties in the LBNL UZ Flow Model appear the same for all the calibrated UZ flow fields considered in the TSPA-VA base case analysis [Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998, (tables 2-19 through 2-23 and tables)]. This approach fails to reasonably bound the uncertainty in the distribution of UZ flow between rock matrix and fractures. Additionally, using the F/M reduction factor as the sole model calibration parameter for the base case flow fields results in the false conclusion that the assumed fracture hydraulic properties have little effect on predictions of repository performance.

- The fast-path contributions to flow, as suggested by geochemical data, are not adequately represented in the site-scale model. This is likely a model artifact caused by the assumption of homogenous model layers and volume averaging matrix and fracture properties over the model grid.

2.3 PATHS TO RESOLUTION

The concerns in the previous section can be addressed through the following paths.

- DOE should continue with plans to perform 3D model calibrations.

- It should be demonstrated that values assigned to fracture continuum hydraulic properties, α_f and m_f, are consistent with the distribution of fracture aperture sizes. Additionally, fracture data used in such a demonstration should be corrected to account for the under-representation of fractures that intersect the ESF at low angles.

- The variety of UZ flow fields generated from the LBNL UZ Flow Model for use in TSPA analyses should fully bound the distribution of mass flux between rock matrix and fractures by accounting for the uncertainty in rock matrix properties and potential biases in borehole saturation profile measurements.

- Although volume-averaging approaches may be adequate for site-scale flow calculation, alternative models should be used to confirm the results or to confirm the parameters used to run the site-scale model. In the latter case, the use of alternative models would be used to scale up properties to the cell sizes used in the site-scale model. Additionally, the LBNL UZ Flow Model should account for heterogeneity or discrete features that result in fast flow through the PTn layer, so that modeled flow rates are consistent with geochemical evidence for fast transport to the repository horizon.

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3 INFILTRATION AND FLOW ABOVE THE REPOSITORY HORIZON

Processes that control the flux and distribution of water reaching the repository horizon at YM are divided into two categories: shallow infiltration and deep percolation. Shallow infiltration at YM is affected by several spatially variable factors, including local precipitation, surface runoff, evaporation, plant transpiration, soil type and depth, and underlying bedrock geology. Shallow infiltration may also vary considerably with time. Precipitation events that cause enough shallow infiltration to escape the rooting zone, hence, becoming deep percolation, are thought infrequent; several years may pass between such events. Over much longer time scales, climate cycles between glacial and interglacial periods are also expected to affect shallow infiltration.

Deep percolation, which refers to the flow of water from the near surface environment to the water table, is influenced by the hydrogeology of the UZ at YM. The temporal and spatial variability of shallow infiltration may be significantly attenuated by deep percolation processes. For example, the porous, relatively unfractured PTn may slow down and spread out large, localized, fast-moving shallow infiltration pulses that arrive via fracture pathways in the densely welded Tiva Canyon layers that outcrop at the surface of YM. As discussed in the following sections, however, it is believed that pathways may exist for a portion of infiltrating water to effectively bypass the PTn layer and move quickly to the repository horizon.

NRC staff previously reviewed site characterization data and DOE modeling approaches to both the shallow infiltration and the deep percolation subissues (Nuclear Regulatory Commission, 1998). The following sections provide an update to previous reviews with a focus on the DOE treatment of these subissues in the TSPA-VA documents (Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998; U.S. Department of Energy, 1998).

3.1 REVIEW OF U.S. DEPARTMENT OF ENERGY APPROACH TO TOTAL SYSTEM PERFORMANCE ASSESSMENT FOR THE VIABILITY ASSESSMENT

The approach for calculating flux at the repository horizon presented in the TSPA-VA is substantially different from approaches adopted in previous DOE PAs. Previous approaches used a pattern of mean annual infiltration (MAI) that changed over a glacial cycle with little physical basis. The TSPA-VA approach is more physically based, linking postulated changes in mean annual precipitation (MAP) to MAI through the use of 1D 100-yr simulations applied on a grid with 30-m × 30-m elements. The calculated MAI for each element is used to create a site-scale MAI map of the YM region (Flint et al., 1996). The 1D fluxes from the MAI maps are then converted to flux boundary conditions for the 3D Site-Scale Unsaturated Zone Model of YM (Bodvarsson et al., 1997), assuming steady-state infiltration. This enables direct simulation of deep percolation fluxes at the repository horizon. These repository-horizon fluxes are used to predict seepage into drifts, as discussed in chapter 4.

The 1D simulator used to link climate to MAI is a bucket model (Flint et al., 1996). In the bucket model, daily rainfall is assumed to enter the subsurface until the soil holding capacity is exceeded, with excess rainfall running off (applied independently as channel flow). Soil moisture is assumed to pond on the soil/bedrock interface, draining by gravity into the bedrock and fracture system while evapotranspiration returns water to the atmosphere. Explicit consideration of lateral flow (overland or subsurface) is not considered for the models used to support the TSPA-VA, aside from applying runoff within channels.

However, DOE made efforts toward developing and testing a coupled surface runoff module for the TOUGH2 code used in the LBNL UZ Flow Model (Bodvarsson et al., 1997, chapter 9).

Linkage of MAI to climate change is handled solely through changes in MAP, with present-day mean annual temperature (MAT), vegetation, and soil characteristics assumed constant throughout the performance period. The methodology used by the DOE predicts the largest values of MAI on ridge tops and side slopes due to shallow soils overlying fractured bedrock, while little or no MAI is obtained in areas with deep soils (e.g., alluvium-filled wash bottoms). Independent simulations predict broadly similar patterns of MAI. However, it remains to be demonstrated that considering only changes in MAP bounds the effects on MAI of changes in all climate-related factors.

For comparison of 1D simulation results to other estimates of percolation flux, it is convenient to calculate area-averaged infiltration from the MAI maps. However, the calculated area-average MAI depends on the area under consideration. For example, consider the following average net present-day MAI values when calculated for the following three important areas of the DOE infiltration map (Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998):

- Over the entire infiltration model of Flint et al. (1996)–3.8 mm/yr
- Over the entire LBNL UZ Flow Model (Bodvarsson et al., 1997)–4.9 mm/yr
- Over only the repository horizon–7.7 mm/yr.

DOE investigated numerous lines of evidence to support their modeling estimates of present-day MAI and to bound uncertainty. These include (i) soil moisture in shallow neutron-probe boreholes, (ii) apparent temperature-distribution anomalies in boreholes, (iii) chloride, (iv) ^{36}Cl, (v) tritium and ^{14}C mass balance calculations, (vi) perched-water mass balance calculations and carbonate, and (vii) silicate-deposit thicknesses in fractures exposed by the ESF. These lines of evidence do not materially contradict the 1D simulation predictions, and are generally within a range of MAI of 1–15 mm/yr over the repository footprint.

In both the LBNL UZ Flow Model (Bodvarsson et al., 1997) and the TSPA-VA Technical Basis Document (Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998), DOE cites percolation flux estimates based on borehole temperature data to support the MAI maps generated from the 1D modeling simulations. DOE deems data from certain boreholes unreliable, primarily those from shallow boreholes that may be affected by significant air movement through the soil. Estimates of percolation flux from the 18 boreholes near YM not excluded by DOE range from 0–15 mm/yr [Bodvarsson et al., 1997 (table 11.4)]. Note that the boreholes on YM are typically drilled in areas accessible to a drilling rig, which means borehole locations may be biased to areas that have significant soil thickness. Because U.S. Geologic Survey (USGS) (Flint et al., 1996) and NRC predictions both suggest that most infiltration occurs where soils are thin, the borehole locations may be biased to areas of low infiltration. Additionally, data from two boreholes, NRG-6 and NRG-7, are discarded—ostensibly, because shallow depth was thought to result in biased estimates due to near-surface vapor transport. These two boreholes, with infiltration estimates of 37 and 30 mm/yr, both (i) are at the base of sideslopes where soils are shallow, (ii) are deeper than at least one included borehole, and (iii) have better error estimates than most of the included boreholes. Although vapor transport may skew MAI predictions for these boreholes, it is also possible that MAI is quite large in these locations, given the shallow soil at their locations.

Figure 3-1 shows that the relative frequency of MAI estimates based on data from the included boreholes is fit well by a log-normal distribution with a $\log_{10}$ (MAI) mean value of 0.76 and a standard deviation of 0.36. This distribution yields an average (mean) percolation flux equal to 6.7 mm/yr, based on the equation

$$\log m_y = m_{\log y} + \frac{\sigma^2}{2} \tag{3-1}$$

where m_y is the population mean, $m_{\log y}$ is the mean of the population $\log_{10}$ values, and σ is the standard deviation of the population. One can envision that the estimated mean percolation flux would be significantly higher if the infiltration estimates from NRG–6 and NRG–7 were included.

To assess whether a mean percolation flux of 6.7 mm/yr is consistent with the DOE present-day MAI map, the area covered by the borehole temperature data must be considered. The 18 boreholes used in this analysis are distributed over an area roughly comparable to that covered by the LBNL UZ Flow Model. Thus, the mean percolation flux value of 6.7 mm/yr can be compared to the MAI value of 4.9 mm/yr calculated by DOE (1998) for that area of the present-day infiltration map. This analysis suggests that the DOE map of present-day MAI may slightly underestimate shallow infiltration. However, given the uncertainty in making such estimates, the two estimates are generally in good agreement.

Due to computational limitations related to the LBNL UZ Flow Model, only a limited number of MAI simulations are considered for the TSPA-VA. These few simulations must account not only for climate change but also for uncertainty in model parameters. To account for climate changes, MAI maps representing three climate states are used in the TSPA-VA calculations: (i) present-day, (ii) LTA, and (iii) super-pluvial. For 10,000-yr simulations, the time of a switch between present-day and LTA climates is randomly sampled from a uniform distribution over the 10-ky simulation duration. For million-year simulations, a glacial cycle is assumed to last for 100 ky, starting with present-day conditions and moving to LTA conditions with a random onset time. A super-pluvial condition is only encountered in occasional glacial cycles (every two or four cycles). The length of time applied to present-day and super-pluvial climates is sampled from a uniform distribution over 20 ky, with the LTA climate existing for the remainder of the 100-ky cycle. For the DOE nominal (best guess) case, the area-averaged steady-state MAI fluxes over the repository horizon are

- Present-day climate—7.7 mm/yr
- LTA climate—42 mm/yr
- Super-pluvial climate—110 mm/yr.

It should be noted that these area-averaged MAI values are given for comparison purposes only; in the DOE model, MAI is a spatially variable boundary condition.

To account for uncertainty in model parameters that affect MAI maps, the DOE TSPA-VA model uses multipliers to vary MAI values over a range of one-third to three times those of the nominal case. One of three multipliers (1/3, 1, or 3) is randomly selected for each glacial sequence and applied throughout the sequence. For example, if a multiplier of 3 is selected, the resulting area-averaged flux over the repository horizon would be 23 mm/yr for the present-day, 126 mm/yr for the LTA, and 330 mm/yr for the super-pluvial climates. The range of multiplier values is justified by DOE based on the consistency of internal model predictions and field observations; higher values of MAI are reported to yield site-scale model predictions that cannot be made compatible with field observations.

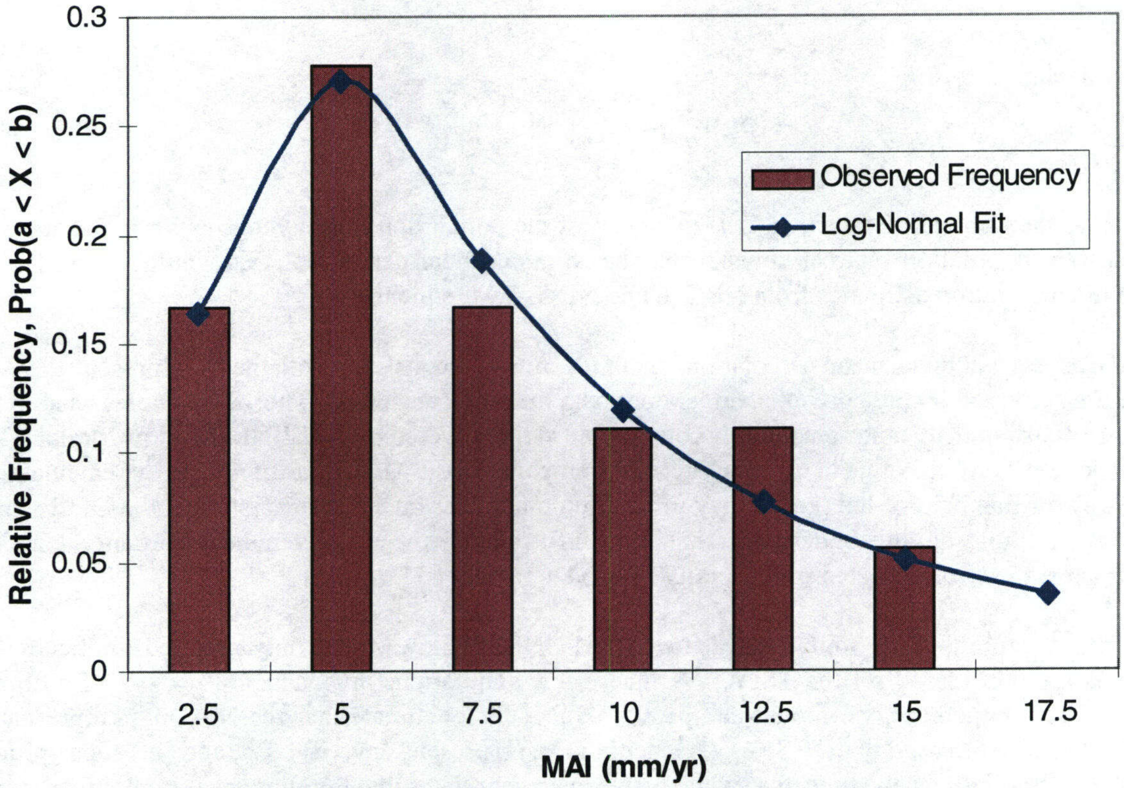

Figure 3-1. This histogram shows the relative frequency of the borehole temperature-based percolation flux estimates of Bodvarsson et al. [1997, (table 11.4)]. A log-normal distribution with a mean $\log_{10}$ (MAI) value of 0.76 and standard deviation of 0.36 provides a generally good fit, yielding an expected value of 6.7 mm/yr.

In the DOE PA model, the three multipliers (referred to by DOE as the *I/3*, I, and *I*3* cases) are assigned probabilities such that, over many model realizations, the average value for MAI at each map element approaches the nominal case value. Although not explicitly stated by DOE, this would require the probabilities be governed by the equation

$$\tfrac{1}{3} p_{I/3} + p_I + 3 p_{I*3} = 1 \tag{3-2}$$

where p_i is the probability that multiplier i will be selected. In the TSPA-VA, *I*3* is assigned a probability of 0.10. From Eq. (3-2) and the fact that the sum of probabilities must equal 1, the probability of 0.30 must be assigned for the *I/3* multiplier and 0.60 for the I multiplier.

According to the TSPA-VA Technical Basis Document (Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998), the probabilities assigned to MAI multipliers are based on "...balancing the recommendations [of] participants in the UZ Flow Expert Elicitation [Civilian Radioactive Waste Management System, Management & Operating Contractor, 1997 (table 3-1)] with information such as temperature gradient implications [Bodvarsson et al., 1997, (chapter 11)]." From an objective reading of these two referenced documents, the reasoning behind the probability assignments is not transparent. Additionally, in tables 3-1 and 3-2 of the referenced UZ Flow Expert Elicitation, the estimated mean present-day deep percolation fluxes over the repository horizon tend to be somewhat higher (e.g., a 10.3 mm/yr aggregate estimate) than the mean of the present-day MAI map used by DOE (7.7 mm/yr).

Based on this aggregate expert evaluation, it may be prudent to assign a greater probability to the *I*3* case. However, an attempt to do so reveals that the logic behind the multiplier-probability assignments is fundamentally flawed and biased toward producing many realizations with low values of MAI. For example, if the *I*3* case is assigned a probability of 0.15 rather than 0.10, then from Eq. (3-2), the *I/3* case must be assigned a probability of 0.45, which is greater than that of the base case, even though the base case is supposed to represent the best guess. If, however, the probability assignment were conditioned such that the expected value of the logarithm of MAI is equal to the logarithm of the nominal case value, the logic would be consistent. In other words, for the multipliers used by DOE, Eq. (3-2) should be replaced by

$$p_{I/3} \log \tfrac{1}{3} + p_I \log 1 + p_{I*3} \log 3 = 0 \qquad (3\text{-}3)$$

Because the log of 1 equals to zero, and the $\log_{10}$ of 1/3 equals to the negative log of 3, it follows that the values assigned to $p_{I/3}$ and p_{I*3} should be equal.

An important assumption in the DOE model of flux to the repository horizon is that of steady-state infiltration during a given climate cycle. This assumption is justified by DOE because modeling has shown that the rock matrix of the PTn layer, which lies between the surface and the repository horizon, has the capacity to absorb short-duration infiltration pulses of relatively large volume, thereby spreading out and slowing down focused infiltration. However, available geochemical evidence indicates that a significant fraction of deep percolation to the repository horizon may effectively bypass the PTn layer. For example, Bodvarsson et al. [1997, (chapter 15)] examined chloride chemistry data from matrix pore waters and perched waters: they report that relatively high chloride concentrations in PTn pore waters may indicate that most infiltrating water travels vertically through discrete high permeability pathways, or under regions of high infiltration, and other parts of the PTn have older water that is replaced at a much slower rate. Additionally, their 3D chloride transport modeling indicates that chloride concentrations in perched waters are indicative of infiltration rates much higher than modern day. In other words, waters with low chloride concentrations, generally associated with high infiltration rates, may effectively bypass the PTn layer. This concept is supported by observations of bomb-pulse ^{36}Cl along the north ramp and main drift of the ESF that indicate chloride migration from the surface to the ESF may occur in time periods of 40 yr or less.

The 3D LBNL UZ Flow Model used by DOE explicitly models stratigraphic layer offset that occurs near faults. Although, this layer offset allows the model to simulate the focused deep percolation that may occur at such features, the assumption of a homogenous unfractured PTn layer still results in all model flow passing through the PTn layer and the subsequent attenuation of fast-moving infiltration pulses. Thus, the potential implications of ubiquitous fast flow paths over the potential repository are not considered by DOE. In the following section, alternate conceptual models for shallow infiltration and deep percolation are discussed—including mechanisms for UZ flow bypassing the PTn layer.

3.2 REVIEW OF ALTERNATIVE CONCEPTUAL MODELS

Independent calculations of shallow infiltration and deep percolation performed by the NRC are broadly consistent with DOE predictions of the spatial distribution of infiltrating waters. However, NRC calculations support an area-averaged infiltration flux that is nearly twice as high as that estimated by DOE. These NRC calculations are supported by available perched-zone data apparently not considered by DOE. Because the perched zone captures and mixes flows from all vertical pathways through the repository footprint, the perched zone geochemistry represents an average over much larger volumes than can be observed with boreholes in unsaturated areas. Consequently, the perched waters below the repository are a particularly valuable source of data for calculating MAI. If the perched-water data accurately predict MAI through the repository footprint, DOE base case estimates of MAI may be too small by roughly a factor of 2 (7.7 mm/yr as opposed to approximately 16 mm/yr in the repository footprint). Accordingly, TSPA-VA analyses using the upper-bound estimates for MAI (i.e., the *I*3* case) may be more representative of actual conditions at YM.

NRC estimates of MAI are reported in the Issue Resolution Status Report (IRSR) on Unsaturated Zone Hydrology (Nuclear Regulatory Commission, 1998). These estimates are based on the perched zone geochemistry that suggest the areal average MAI is between 7 and 26 mm/yr, with 88 percent of data values yielding local estimates of MAI between 13 and 26 mm/yr. Similarly, calculations by Fabryka-Martin et al. (1997) yielded a range of MAI between 11 and 23 mm/yr and an average of 16 mm/yr.

A key assumption in these calculations is that all pathways for chloride transport converge in a well-mixed perched zone under steady-state fluxes. A combination of long residence times for water in the perched zone and a high fracture density supports this assumption. As noted by Bodvarsson et al. [1997 (chapters 13 and 15)], the waters in the perched water zone are thought to have an average age between 2,000 and 7,000 yr, based on postglacial $\delta^{18}O$ and δD isotopic values, ^{14}C water residence times, and lack of equilibrium with ^{14}C in the gas-phase overlying units. Such long residence times should be sufficient for equilibrium to occur between matrix and perched waters, considering that fracture spacing in the perched zone is estimated less than 1 m [Bodvarsson et al., 1997 (chapter 7)]. It should be noted, however, that disequilibrium between perched zone and matrix pore waters is reported at borehole UZ–14 (Yang et al., 1996). The disequilibrium at UZ–14 has been attributed to emplacement of borehole fluids during drilling of UZ–1 [Bodvarsson et al., 1997 (chapter 15)]. Thus, if perched waters at UZ–14 had not been contaminated, the infiltration estimate would presumably have been higher. Because perched waters are representative integrated infiltration over a relatively large area (compared to boreholes), the larger MAI estimated from the perched waters (e.g., the mean value of 16 mm/yr) is a more a reliable estimate for present-day, area-averaged MAI.

As discussed in the previous section, the Flint et al. (1996) base case MAI map, with an average of 7.7 mm/yr within the repository footprint (4.9 mm/yr over the entire LBNL UZ Flow Model), is used to provide the estimate of MAI for the TSPA-VA (corroborated through numerous independent data sources). Using a similar but independent approach, current NRC infiltration model estimates for area-averaged MAI over the repository footprint are in the range of 15–20 mm/yr. The experience of the authors suggests that numerical simulations can provide useful information on spatial distributions and response to changes in environmental variables, but calibration is required to provide a firm estimate for MAI. NRC infiltration modeling suggests that changing uncertain input parameters within reasonable bounds can change MAI estimates by far more than a factor of 2. For example, soil thickness is a parameter that can have significant impact on MAI; decreasing soil thickness results in increased MAI. In the simulations used to support the TSPA-VA, the minimum soil thickness is 50 cm; however, field experience suggests that soil is often much thinner over the repository footprint. Simply replacing the soil thickness map with more realistic values would likely significantly increase predictions of MAI.

The primary objection to the higher estimate is that consistently lower estimates for MAI are obtained using other data sources. However, the DOE relies most heavily on borehole-based methods to argue that their MAI maps are reasonable. A single grid block in the DOE MAI map typically covers an area 1–3 orders of magnitude greater than the area covered by an individual borehole sample. The collection of borehole-based MAI estimates are generally in the range of 1–10 mm/yr, significantly smaller than the estimates based on the perched water. Estimates representing lower bounds, such as MAI estimates based on fracture fillings exposed within the ESF (roughly 2 mm/yr), or those that can easily be made consistent with MAI values greater than 10 mm/yr, such as the simulations based on ^{36}Cl observations in the ESF (Fabryka-Martin et al., 1997), are not considered further.

When using borehole-based estimates of percolation flux to infer MAI, the DOE does not explicitly assume any particular statistical distribution for flux. However, it is tacitly assumed that the collection of observations should bound the actual value of area-averaged MAI. With sufficient numbers of observations, this argument is valid for any type of statistical distribution. However, when the number of observations is sparse and drawn from a positively skewed (e.g., log-normal) distribution, it is likely that area-averaged MAI is larger than the sample mean, and possibly larger than any of the observations. Because MAI estimates based on perched-water chemistry encompass a much larger sample area, they may be more representative of actual values of MAI. The generally lower estimates of MAI from borehole observations can be explained if the distribution of MAI at the borehole scale is log-normal, which is supported by the distribution of temperature-based estimates shown in figure 3-1. Additionally, repository-horizon flux distributions presented for the present-day climate by Bodvarsson et al. [(1997 (section 20.6)] are positively skewed and might easily be described by a log-normal distribution; note that, due to averaging, the distribution of fluxes at the grid scale is likely considerably narrower (less skewed) than at the borehole scale.

For any log-normally distributed variable with nonzero variance, the mean of the distribution is larger than the median. Thus, it is reasonable to expect the majority of borehole-based MAI estimates will be less than the mean value. When the variance is sufficiently large, the true population mean (m_y) is expected to be larger than the arithmetic mean of the sample distribution. For example, using the corrected percolation flux estimates from 18 boreholes provided in table 11.4 of Bodvarsson et al. [1997, (chapter 11)], the sample mean percolation flux is about 5.9 mm/yr. However, as shown in figure 3-1 and discussed in the preceding section, a population mean of 6.7 mm/yr is obtained by fitting a log-normal distribution to a relative frequency plot of these borehole-based estimates. An area-averaged MAI of 6.7 mm/yr is somewhat larger than the value of 4.9 mm/yr estimated for roughly the same area of the DOE present-day MAI map —even ignoring the fact that borehole locations may be biased toward areas with lower infiltration. Based on the foregoing discussion, an area-averaged MAI of 16 mm/yr over the repository horizon, consistent with the Fabryka-Martin et al. (1997) perched water chloride chemistry-based estimate, is not inconsistent with the lower borehole-based estimates when the sample area is considered.

As recognized by the DOE, it is difficult to reconcile the high values of MAI implied by the perched waters with observations of the PTn unit. The PTn unit is generally considered a strong homogenizing unit, capable of strongly damping or eliminating wetting pulses in the fracture system due to the large matrix storage capacity and capillary attraction from fractures into the matrix. Because of this strong damping capacity, the matrix fluxes in the PTn are thought representative of MAI. However, NRC (1998) calculations suggest that only a small fraction (less than 10 percent) of the waters in the perched-water system can originate as waters in the PTn matrix if chloride mass balance is to be obtained. This observation is in direct contradiction to the hypothesis that the PTn unit eliminates essentially all fast-path flux, and calls into question the assumption that the PTn is a barrier to wetting pulses.

Several plausible mechanisms allow waters to reach the perched zone without being observed in the PTn matrix samples. The most plausible source of water for the perched zone is net infiltration, generally within and somewhat to the north of the repository footprint; lateral-flow sources (e.g., Solitario Canyon, lateral flow in the perched zone) are not considered further. The preferred DOE explanation, also arrived at by the UZ Flow Expert Elicitation Panel (Civilian Radioactive Waste Management System, Management & Operating Contractor, 1997), is that a combination of fractures and small faults in the PTn allows the waters to bypass the matrix, perhaps with coatings insulating the matrix from the fractures. This combination is quite possible, but direct observation of PTn fractures (Sweetkind et al., 1997) provides little evidence of fracture flow or fracture coatings. Further, the fracture systems tend to be strata-bound, so that connection between the fracture systems in different units is greatly reduced. Accordingly, this theory most plausibly requires that waters would pass through the PTn in numerous small unmapped faults. Relatively small amounts of lateral down-dip movement would occur with this hypothesis.

An alternative hypothesis achieves essentially equivalent effects without invoking fracture flow through the PTn. The PTn is not homogeneous, and the PTn core samples have considerable variability within each subunit. It is quite plausible that fine-scale matrix heterogeneity provides localized fast pathways within the matrix that are sufficiently infrequent that no borehole has yet penetrated a pathway. The arguments regarding skewed flux distributions made previously would apply here as well, so that area-averaged matrix fluxes are likely higher than most or all observations. Probably relatively small amounts of down-dip movement would occur with this hypothesis.

Another alternative hypothesis is that down-dip lateral diversion could occur at the top of the PTn unit. Down-dip diversion occurs when a permeability or capillary barrier is reached. A capillary barrier is achieved when a fine-grained medium overlies a coarse-grained medium. A permeability barrier is achieved when a high-permeability medium overlies a low-permeability medium. Both types of barriers occur at the PTn, with a capillary barrier occurring between the bottom of the Tiva Canyon welded (TCw) matrix and PTn matrix, and a permeability barrier occurring between the bottom of the PTn matrix and the Topopah Springs welded (TSw) matrix. Early analyses indicated that substantial down-dip movement was possible due to the permeability barrier at the bottom of the PTn providing an umbrella over the repository that may divert substantial water into faults. Analyses using more recent hydraulic parameters show significantly reduced lateral diversion. However, these analyses typically have not considered lateral diversion in the TCw fracture system overlying the PTn. It is entirely possible, however, for significant lateral diversion to occur at the bottom of the highly permeable TCw fracture system due to a permeability contrast between fractures and matrix, particularly if fractures are strata-bound within the welded units. Note that fracture-system diversion in the TCw unit may be larger than would be predicted by the steady-state analyses performed by DOE (Bodvarsson et al., 1997) because permeability-contrast diversion is enhanced as fluxes increase, and the episodic fluxes in the TCw may be orders of magnitude larger than the time-averaged fluxes. Lateral diversion may focus significant fluxes into fault zones, enabling much of the MAI fluxes to bypass the PTn matrix through narrowly focused zones.

It is likely that all these previously noted mechanisms for bypassing the PTn are active to some extent. The balance between the mechanisms has implications for repository performance: if lateral flow dominates, substantial protection may be offered to the repository. The simulations in the TSPA-VA do not include strata-bound fractures in the flow model; this results in predictions of primarily vertical flows through the PTn. Thus, the TSPA-VA simulations are conservative for channeling MAI fluxes through the repository footprint. Although some lateral diversion is plausible, significant independent evidence for lateral flow would be required to accept credit for simulations with significant lateral diversion above the repository footprint.

3.3 SUMMARY OF CONCERNS

The overall approach in the TSPA-VA provides a reasonable starting point for calculating fluxes at the repository horizon.

- The authors agree that the use of MAI multipliers, used to incorporate uncertainty in MAI estimates into the TSPA abstraction, is reasonable. However, the methodology for calculating the probabilities assigned to MAI multipliers is biased toward producing low values for MAI.

- Integration of all sources of data used to estimate MAI, including perched-water data, and the natural variability of these data suggests that the TSPA-VA nominal-case, area-averaged MAI may be too low by approximately a factor of two.

- DOE has not demonstrated that climate-related changes in temperature, vegetation, and soil can be neglected while still providing a reasonably conservative bound on infiltration under future climates. This concern stems from the fact that decreases in temperature can result in increased infiltration, even when precipitation does not change. Although this effect may be limited by increased vegetation, the interplay between these factors has not been investigated. Further, observations of soil thickness and texture on YM indicate these properties have been significantly different in the past. If it can be shown that the overall impact of these effects is minor relative to changes in precipitation, then the present method is acceptable.

- DOE has not demonstrated that neglect of overland and shallow subsurface lateral flow provides a conservative bound on MAI. These neglected lateral flow processes may significantly increase MAI in certain areas, or create fast, high-flux pathways due to focused flow. The resulting alternate patterns of MAI would change the distribution of fluxes at the repository, which could alter drift seepage calculations.

- The assumption of steady-state infiltration fluxes in the LBNL UZ Flow Model precludes an assessment of the impact of episodic infiltration that may bypass the PTn layer and travel quickly to the repository horizon. In the TSPA-VA [U.S. Department of Energy, 1998 (volume 1)], the DOE acknowledges that as much as 80–90 percent of infiltration may bypass the PTn layer via fast pathways. Flow in these fast pathways is likely to be episodic, and such transient flow is more likely to result in seepage into repository drifts.

3.4 PATHS TO RESOLUTION

The concerns in the previous section can be addressed through the following paths:

- DOE could use an unbiased methodology for assigning probabilities to MAI sample values [e.g., Eq. (3-3)].

- DOE could resolve contradictions between independent estimates of MAI by incorporating estimates of MAI based on perched water geochemistry and accounting for the apparent positive skew in the statistical distribution of the borehole-based, deep percolation estimates into a consistent estimate of area-averaged MAI.

- It should be demonstrated through simulation or observation of analog sites that considering only changes in MAP bounds the effects on MAI of changes in all climate-related factors.

- Infiltration modeling should account for overland and shallow subsurface flow, which are likely to change the calculated patterns of MAI by lowering predictions at topographic high points and increasing predictions at topographic low points. This concern can be addressed through two-dimensional (2D) or 3D simulations of infiltration along hill slopes. Alternatively, a demonstration that the patterns of MAI have little effect on flux patterns at the repository horizon will address the concern regarding seepage statistics.

- The DOE UZ flow model should include features that allow rapid transient percolation to bypass the PTn layer. The impact of these transient pulses on seepage into repository drifts could then be examined.

4 PERCOLATION FLUX AT THE REPOSITORY AND DRIFT SEEPAGE

In both DOE (1998) and NRC studies (1999), the amount of water contacting WPs has consistently been identified as one of the most important parameters affecting performance of the proposed HLW repository at YM, as gauged by the amount of predicted radionuclide migration via groundwater pathways. Early in the life of a proposed repository, heat generated by the emplaced WPs is expected to cause a dry-out zone surrounding the repository drifts that may offer protection of WPs from percolation fluxes for a limited time period. Eventually, as the heat generated by WPs declines, a return to ambient percolation fluxes is expected. However, by that time, thermal alteration and mineral deposits left behind by evaporating water may have altered the near-field flow system in ways not understood. For example, minerals may fill voids in the fracture networks surrounding the drifts, resulting in increased protection from dripping. On the other hand, thermal expansion and contraction may result in the widening of fissures or even the collapse of repository drifts onto WPs.

The number of WPs expected contacted by water is a function of two important factors (i) the areal distribution of percolation fluxes reaching the repository horizon that could potentially result in seepage into the drift cavity and (ii) the amount of seepage exclusion from drifts (around or down the walls of the open drift space) due to capillary forces in the fracture and rock matrix flow systems. Several maps of the expected percolation flux at the repository horizon were created by DOE researchers to account for a number of parameter sets meant to bound the uncertainty in the UZ flow system above the proposed repository horizon. The factors that affect the development of such maps were reviewed in the preceding section and concerns were identified. In this chapter, the technical review focus is on the DOE conceptual models and approaches for modeling seepage exclusion of water from drift cavities.

4.1 REVIEW OF U.S. DEPARTMENT OF ENERGY APPROACH TO TOTAL SYSTEM PERFORMANCE ASSESSMENT FOR THE VIABILITY ASSESSMENT

The DOE uses a single porous media continuum approach for modeling the seepage of deep percolation into drifts. In this model the network of intersecting fractures in the welded tuff of the proposed repository horizon is treated as a continuous porous medium, and flow is averaged over a representative elementary volume (REV) of the porous medium. Similarly, the properties controlling flow (i.e., permeability and moisture retention characteristics) are also averaged and represent the bulk properties of the REV rather than properties of individual fractures. Because there is no consensus as to what scale or under what conditions flow through fractured rock is analogous to flow through porous media, a greater and perhaps more substantial weakness of the DOE seepage model is the lack of data regarding the bulk hydraulic properties of the fracture continuum. Particularly notable, and perhaps of greatest concern, is the near total absence of data on the drift scale hydraulic properties of the Topopah Springs lower lithophysal unit (Tptpll) in which most of the WPs would be placed.

At present, the only direct measurements of fracture properties that affect drift seepage are air permeability and fracture frequency in the middle nonlithophysal unit—performed to support the drift scale heater test and niche seepage studies. From these data the moisture retention characteristics and structure of spatial heterogeneity of fracture continuum properties have been estimated. While air permeability measurements may adequately characterize some scales of spatial heterogeneity, their use in determining moisture retention curves is certainly novel, unproven, and dependent upon several unsubstantiated assumptions. For example, the van Genuchten alpha parameter for fractures (α_f) was estimated from effective fracture apertures using the equation

$$\alpha_f = \frac{b\rho g}{2\tau\cos\theta} \tag{4-1}$$

where b is the fracture aperture, ρ is the density of water at 20 °C, g is the gravimetric acceleration constant (9.8 m/s^2), τ is the surface tension of water at 20 °C, and θ is the contact angle of water with the mineral surface (assumed to equal zero, thus cos θ = 1) {[Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (chapter 2, Eq. (2-5)]}. It must be recognized, however, that such an approximation at best, can be regarded as no more than an order-of-magnitude approximation. Additionally, direct measurements of capillary pressure and saturation relationships of a single fracture (Reitsma and Kueper, 1994) indicate that air entry pressure and the reciprocal of the van Genuchten α_f fitting parameter may differ significantly.

Other tenuous assumptions used in the DOE drift seepage model include: use of air permeability as a proxy for bulk intrinsic permeability of fractures for water; derivation of effective fracture apertures from the cubic flow law and use of apertures to estimate the van Genuchten α_f parameter, and the assumptions that fracture density is uniform and small fractures (e.g., less than about 0.5 m) are not important. Model uncertainty accumulating from these assumptions and approximations is not adequately addressed in the TSPA-VA, particularly in light of model sensitivity to the α_f parameter of the moisture retention curve. (Sensitivity of the critical, or threshold, percolation flux to permeability and the α_f parameter is discussed in the supporting analyses contained in the following section.)

The DOE seepage models deal with uncertainty in the parameter by using a range of possible values in their simulations. That this range of values encompasses the range of uncertainty and heterogeneity in the moisture retention characteristics of the fracture network in the repository formation, however, is not conclusively demonstrated. In particular, the presence of asperities, or surface roughness of the drift crown, and discrete fractures dead-ending at the drift crown would result in much less effective capillary retention and more seepage into the drifts for a given percolation flux.

In the DOE seepage model simulations (e.g., Wang et al., 1998; Tsang et al., 1997), heterogeneity in the hydraulic properties of the repository formation fracture network is a dominant factor and yet is considered only for permeability, while the moisture retention parameters and porosity are treated as spatially uniform. Arguments are given as to why using a spatially uniform α_f parameter is a conservative assumption (Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998); however, no supporting evidence or model sensitivity studies are presented. A combination of low permeability and large α_f parameter will result in little seepage exclusion or capillary diversion, even at low percolation fluxes. This could possibly occur in a situation where a low density of fractures has variable apertures.

The DOE fracture continuum model is also sensitive to the correlation scale of heterogeneity. Heterogeneity exists in YM on multiple scales and yet is treated in the seepage models only on the scale of air permeability measurements and the scale of possible discrete fractures intercepted by the drifts. Thus, two fairly similar scales of heterogeneity for one parameter are expected to represent all the multiple scales of heterogeneity, from potential focusing of infiltration into preferential paths on the mountain scale down to surface roughness of the drift crown on a micro-scale. It is difficult to believe that heterogeneity in permeability on the scale of a few meters adequately represents all the variability controlling seepage into open drifts.

A final concern is the method of abstracting seepage models into the PA may result in biased results. There is, for example, no basis on which the weights to various parameters are assigned. Assigning a weight of 50 percent to the mean α_f value and a weight of 25 percent to the order of magnitude extremes is arbitrary. Further, irregularities of the drift crown surface that are not accounted for in models probably make assigning a larger weight to the larger value of α_f appropriate. Additionally, the DOE TSPA-VA abstraction approach does not consider the effects of transient flow, which are shown important in the seepage modeling analyses (e.g., Tsang et al., 1997).

In summary, heterogeneity appears to be the single most important factor controlling the estimation of seepage into drifts. Yet heterogeneity of a single parameter (i.e., intrinsic permeability of a fracture continuum on the scale of a meter or so) is expected to account for heterogeneity on multiple scales: from the mountain scale, where infiltration is averaged over large areas in the DOE models, down to the scale of roughness of the drift crown, which is not resolved by the DOE models. On the larger scale, the estimation of seepage is potentially biased by averaging infiltration over large blocks. Using the mean percolation flux over a subarea of the mountain scale to estimate the percolation flux necessary to induce seepage at the drift scale may result in significant underestimation of both the seepage flux entering the drifts and the fraction of WPs contacted by liquid water. On the small scale of a driftwall, the presence of surface irregularities and conducting fractures that dead-end at the drift crown will result in less capillarity, and thus less diversion, of percolation flux around the drift. For the drift-scale fracture continuum model, the effect of this small-scale heterogeneity could be accounted for by using larger effective alpha parameters for model grid blocks representing the driftwall; this would account for the additional seepage caused by these irregularities. Neglecting the multiple scales of strongly anisotropic heterogeneity and arbitrarily assigning the most weight to the mean alpha parameter instead of the larger effective alpha parameter, which actually controls capillary retention and seepage near the drift crown, results in a biased and nonconservative abstraction of both quantity of seepage into drifts and fraction of WPs wetted by dripping.

The strongest evidence supporting the applicability of a fracture continuum approach to modeling drift seepage comes from the liquid injection niche studies (Wang et al.,1998) conducted in the ESF. A fracture continuum model was able to effectively match the results of the experiment using α_f as a calibration parameter (modified from 1/1,000Pa to 1/20Pa). However, flow in the liquid injection tests occurred over a length scale of less than one meter and at rates greatly in excess of naturally occurring percolation. Additionally, permeability estimates at the liquid injection boreholes, based on air injection tests before and after niche excavation, indicated a nearly two orders of magnitude, post-excavation increase Wang et al., 1998). Thus, the assumption of a fracture continuum may have been appropriate for the niche studies only because of the increased fracturing resulting from niche excavation. Alternatively, the higher post-excavation permeability estimate may reflect a bias in the estimation method due to the unaccounted for presence of the niche cavity acting as a boundary condition. If the latter case is true, then the permeability value used by Wang et al. (1998) to match model results to the fluid injection results may have been two orders of magnitude too high. Given the possibly biased results of this single niche study, the applicability of a fracture continuum approach to modeling seepage into drifts has yet to be effectively demonstrated. Ongoing infiltration and seepage studies being conducted in Alcove 1 of the ESF may be useful in this regard.

The applicability of the DOE conceptual model for drift seepage is also challenged by the long time period between the early dry-out conditions and the return to ambient percolation fluxes. By this time an open drift would likely have experienced at least partial collapse and the WPs may be buried in rock debris. Should some cavity remain, it is unlikely that it would have the same geometric relationship to the WP as in the DOE seepage model. Under such conditions, the DOE model of capillary diversion around open drifts may be irrelevant.

Due to thermal effects, long-term, perhaps permanent, changes in the repository formation hydraulic properties are also possible. Mineral precipitation, dissolution, or both may cause filling or enlarging of fractures, thus altering both permeability and moisture retention characteristics of the fracture continuum. Under these conditions, the range of hydraulic parameters used in the DOE seepage model may be no longer representative. Whether the changes in fracture hydraulic properties result in increased diversion of flux away from the WPs or focusing of flow toward the WP due to heterogeneity is largely uncertain. These near-field alteration factors should be taken into consideration, and the uncertainty involved should be accounted for in the PA.

4.2 KEY PARAMETER SENSITIVITY ANALYSIS OF U.S. DEPARTMENT OF ENERGY DRIFT SEEPAGE MODEL

Sensitivity of seepage exclusion from an underground cavity to permeability and the van Genuchten α_f parameter (van Genuchten, 1980) is illustrated in this section using a single-continuum unsaturated flow model with both analytical and numerical solutions. For this analysis, cavity geometry is a flat-topped strip 1-m wide. Shown in figure 4-1 is the 15- × 20-m model domain and grid used for the numerical solution with MULTIFLO Version 1.2β (Lichtner and Seth, 1998). The cavity is shown as the small white strip in the central area of the model domain. Grid blocks above and in the strip cavity have vertical dimensions of 2.5 cm, which are not resolved at the scale of this figure and appear as a solid line through the center of the grid. The sides of the model domain are no-flow boundaries, a Dirchlet boundary condition is assigned to the bottom, and a steady-state flux condition representing uniform deep percolation is assigned to the top boundary. The capillary pressure in the cavity is maintained at zero for all saturations.

Sensitivity of the critical percolation flux to permeability and the alpha parameter is shown in figure 4-2. Critical percolation flux is the steady uniform deep percolation rate at which seepage into the cavity is incipient. The filled circle symbols in figure 4-2 are from the analytical solution of Philip (1989) for a strip-shaped cavity

$$q_c = K_s\left(1 - \alpha_G lB\right) \tag{4-2}$$

where q_c is the critical percolation flux; K_s is saturated permeability; l is the half-width of the cavity; α_G is the Gardner alpha (Gardner, 1958), which is analogous to the van Genuchten alpha; and B is calculated from

$$B = \frac{1}{\alpha_G l} - \frac{1}{(\alpha_G l)^3} + \frac{9}{(\alpha_G l)^5} - \frac{225}{(\alpha_G l)^7} + \frac{11025}{(\alpha_G l)^{11}} - \frac{893025}{(\alpha_G l)^{13}} + \ldots \tag{4-3}$$

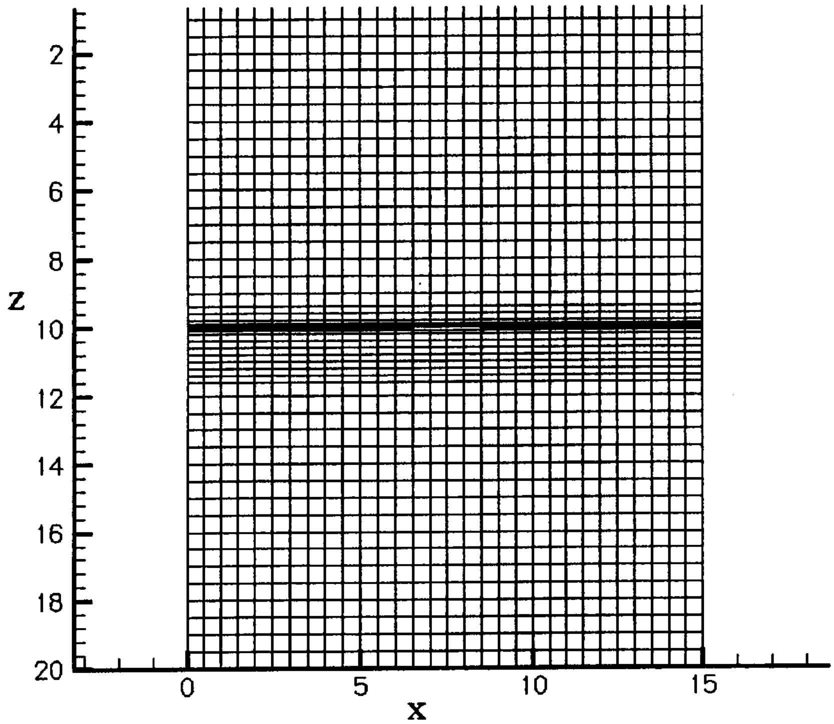

Figure 4-1. Model domain and grid used for numerical solution of critical percolation flux. The strip-shaped cavity is indicated by the white dash in the center. Units for the x and z axes are meters.

The triangular symbols are from steady-state numerical simulations of the critical percolation flux. The solid lines in figure 4-2 indicate a homogeneous fracture continuum permeability of 10^{-13} m^2, the dashed lines indicate a permeability of 10^{-12} m^2, and the dotted lines indicate a permeability of 10^{-14}m^2. In figure 4-2 it can be seen that an order of magnitude decrease in permeability results in an order of magnitude decrease in critical percolation flux. However, an order of magnitude increase in the alpha parameter (either the van Genuchten alpha from the numerical simulations or the Gardner alpha from the analytical solution) results in over two orders of magnitude decrease in the critical percolation flux. Thus, for some van Genuchten alpha parameters within the range considered by the TSPA-VA, there is little exclusion or diversion of percolation flux away from the cavity due to capillary forces.

4.3 REVIEW OF ALTERNATIVE CONCEPTUAL MODELS

A fracture continuum model for capillary diversion of percolation flux away from open drifts assumes capillary dominated flow within individual fractures. The notion of capillary pressure within a fracture approaching zero and saturation approaching one as a prerequisite to seepage into the drift presumes that the fractures are filled with water near the drift. Recent laboratory experiments, however, indicate that gravity driven flow of water in films along the walls of fractures may occur in significant amounts (Tokunaga and Wan, 1997). The mechanisms controlling seepage of fracture film flow into drifts are not addressed in the DOE model, and it is not clear that models of capillary diversion of flow around open drift cavities are applicable if a portion of the percolation fluxes near the rock-drift interface occur as film flow. Failure to

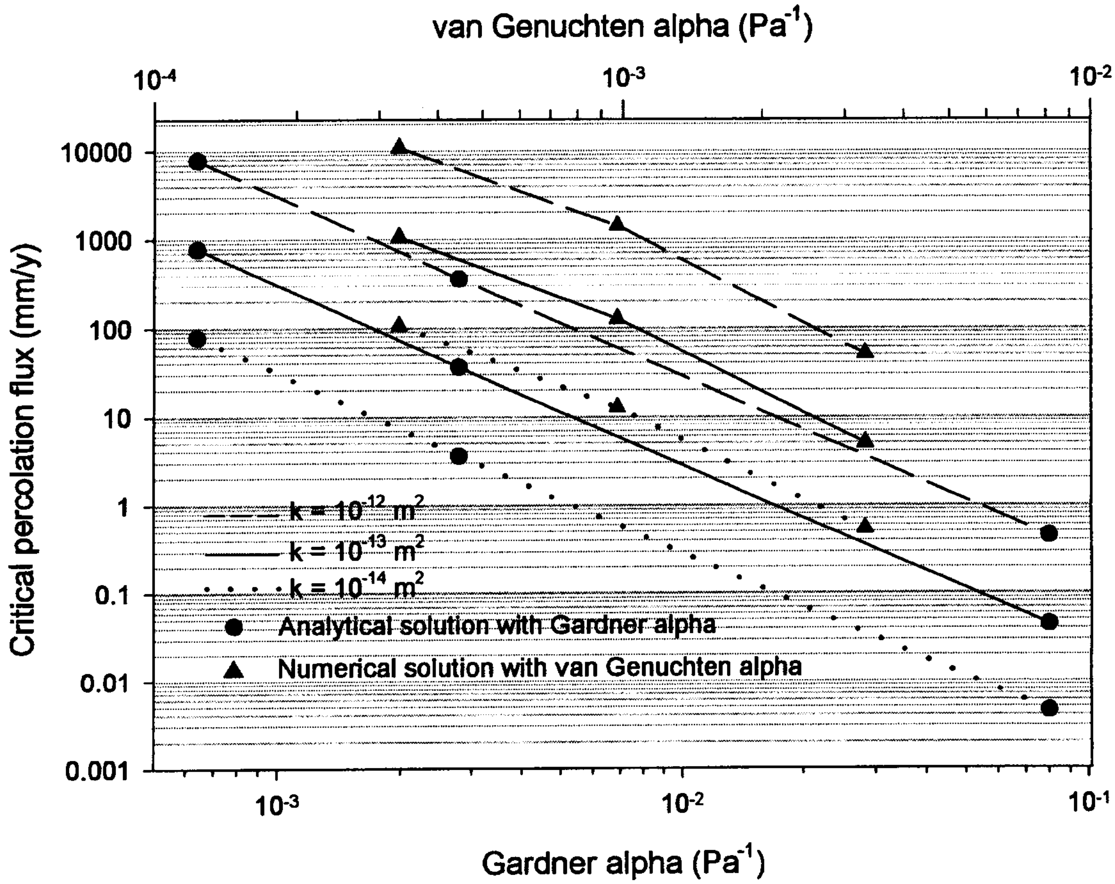

Figure 4-2. Sensitivity of critical percolation flux to permeability and alpha parameters. Filled circle symbols are from the analytical solution of Philip (1989). Filled triangular symbols show the numerical solution of the critical percolation flux using the van Genuchten alpha. Fracture continuum permeabilities of 10^{-12} (dashed line), 10^{-13} (solid line), and 10^{-14} m^2 (dotted line) are indicated.

consider the importance of film flow is a potential weakness in the TSPA-VA, considering the importance of the fraction of WPs contacted by liquid water to repository performance.

A much simpler alternative conceptual model exists that would allow for immediate resolution of the technical concerns regarding drift seepage. That is to assume that all percolation flux that intersects repository drifts will enter as drift seepage, and that all drift seepage that overlies the footprint of a waste canister will contact that canister. This conceptual model is by no means meant to provide an accurate representation of drift seepage and seepage exclusion. It does, however, in the judgment of Center for Nuclear Waste Regulatory Analyses (CNWRA) staff, provide for a conservative estimate of the amount of water that may come into contact with waste canisters. That is, the deviation of the conceptual model from reality will favor predictions of more water contacting waste canisters. This conceptual model also eliminates uncertainties regarding eventual drift collapse, changes in drift geometry, thermal alteration, and the applicability of fracture continuum models.

4.4 SUMMARY OF CONCERNS

The following is a summary of the technical concerns discussed in the previous two sections

- Heterogeneity in the hydraulic properties of the rock that surrounds drift openings may be the single most important factor affecting water flux into open drifts. However, there is no attempt to account for the multiple scales at which heterogeneity occurs, or the resulting uncertainty. Small scale features near the drift crown have a strong effect on seepage, yet little effort is made to include these features either by adjustments to parameters or by incorporating small scale heterogeneity of moisture retention properties. It may never be possible to develop an exact model of seepage drifts, thus, conservative assumptions must be used where uncertainty cannot be reduced.

- Seepage contacting the WPs will be most likely in the time following dissipation of the thermal pulse. By then the geometry of the drifts may have substantially changed due to rockfall, and the properties of the repository formation may have changed due to thermally driven geochemical alteration. Under these conditions, there is little basis for believing the fracture continuum model presented in the TSPA-VA is applicable.

- There is presently no reported data regarding the fracture properties at the scale of concern in the proposed repository formation (i.e., Tptpll). The authors are unaware of any efforts to use facilities such as the East-West Cross Drift to collect this data.

- Weights assigned to ranges of parameters for PA appear to be arbitrary. In addition, PA fails to consider important phenomena such as transient, (episodic) infiltration. As a result of this uncertainty, the quantity of water that would contact WPs may be significantly underestimated.

4.5 PATHS TO RESOLUTION

- If the fraction of deep percolation flux intercepting the areal footprint of the WPs is considered as contacting the WPs, then the issue of diversion of water away from the drifts is resolved.

- Diversion of percolation flux away from drifts and WPs should be supported by data, field studies, and natural analog observations under conditions likely to exist in the repository subsequent to dissipation of the thermal pulse.

- Modeling studies used to demonstrate diversion of percolation flux away from drifts and WPs should be supported by data, account for all sources of heterogeneity and uncertainty, and include coupling to models of drift collapse and alteration of hydraulic properties. Additionally, scoping calculations should be performed to assess the importance of considering the effects of drift collapse and alteration of hydraulic properties.

- The niches and alcoves in the East-West Cross Drift should be allowed to equilibrate to natural conditions by sealing the entrance. This tunnel could then be used as a large-scale test section for evaluating the heterogeneous distribution of percolation across the repository footprint. This would be useful to validate the approach and the parameter estimates used in the LBNL UZ Flow Model and drift-scale seepage models, especially if variability along the drift is measured.

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5 TRANSPORT BELOW THE REPOSITORY IN THE UNSATURATED ZONE

The important processes to be considered for transport of radionuclides from the repository to the water table are dictated by deep percolation flow paths. In the densely welded tuffs that comprise most of the TSw hydrostratigraphic unit below the repository, flow will occur predominantly in the fracture systems. UZ flow patterns through the Calico Hills hydrostratigraphic (CH) unit, below the TSw, are controlled mainly by the extent of welding and zeolitic alteration, which affect both fracture density and matrix permeability. In the LBNL UZ Flow Model, the layer designated as the CH unit is actually composed of alternating nonwelded and welded subunits and several geologic units, including the lower Topopah Springs bedded tuff, Calico Hills Formation[1], Prow Pass Tuff, and Bullfrog Tuff [Bodvarsson et al., 1997(table 3.4-2)]. Within the CH unit, flow in the nonwelded vitric, devitrified, and zeolitically altered horizons will be a mixture of matrix and fracture flow, while flow in the welded horizons will be predominantly in the fracture system. Permeability barriers exist where the fracture system and vitric units overlie zeolitically altered horizons and capillary barriers may exist where the nonwelded vitric overlie welded units. Perched water and lateral flow appear to occur primarily as a result of permeability barriers, as reflected by the widespread presence of perched water at and above the zeolitically altered horizons. The extent of lateral flow is expected controlled by the fracture and fault systems and possibly by the lateral extent of zeolitic alteration.

Because of the importance to predicted repository performance, conceptualizations and parameter values that lead to transport through the matrix of nonwelded units require close analysis. When flow occurs through rock matrix, the increased access to mineral surfaces for radionuclide sorption and reduced flow velocity result in significant delays in radionuclide arrival at the water table. For flow in fractures, RT to the water table is much faster, although matrix diffusion and dispersion may provide some delay in RT. Thus, in the nonwelded units, the fraction of flow that occurs in rock matrix versus fractures is probably the single most import issue for transport—an issue for which there remains considerable uncertainty. For flow that goes through the matrix of nonwelded units, the hydraulic and sorption properties of intermediate rocks may impact dose estimates more than the end member rock types of nonwelded vitric, zeolitic, and devitrified due to the expected flow paths.

5.1 REVIEW OF U.S. DEPARTMENT OF ENERGY APPROACH TO TOTAL SYSTEM PERFORMANCE ASSESSMENT FOR THE VIABILITY ASSESSMENT

The approach DOE uses for flow and transport below the repository to the water table did not significantly change for the TSPA-VA. Steady-state flow fields are calculated using the dual continuum formulation in TOUGH2 and the site-scale LBNL UZ grid. Simulation of RT through the UZ is performed using the FEHMN code and its cell-based variation of conventional particle tracking. The flow fields from the site-scale model passed to the transport model remain at the same scale and hence, do not suffer from the problem of the large jump in scales as noted between the site- and drift-scale models (section 4.1.1).

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[1]To avoid confusion, it should be noted that the Calico Hills Formation is a subpart of the Calico Hills hydrostratigraphic layer. Hydrostratigraphic layers are used to simplify hydrologic models by lumping several stratigraphic layers with similar properties into a single layer.

The DOE UZ transport model uses a more complex subarea delineation than is used in the NRC PA model (Nuclear Regulatory Commission, 1998). In the DOE model, the subareas at the repository level reflect the spatial distribution of percolation, whereas the linkage of subareas to the saturated zone transport model reflects the hydrostratigraphic units intersected by the water table.

In this section, the review focuses on three important transport considerations: (i) flow beneath the repository, (ii) the DOE RT model, and (iii) matrix diffusion in the UZ.

5.1.1 Flow Beneath the Repository

In the current conceptualization of flow patterns, the estimated hydrologic properties of matrix and fractures in nonwelded layers and the resulting partitioning of flow between matrix and fractures are, perhaps, the most important factors controlling RT time to the water table. The partitioning of flow between fractures and matrix used for TSPA-VA transport calculations is determined by dual continua 3D flow fields, generated from the LBNL UZ Flow Model using an assumption of uniform hydraulic properties within each model sublayer.

The use of uniform properties for each sublayer appears to be required to limit the number of parameters considered in the site-scale model calibration process. This is because the flow field below the repository is complex and the hydrologic properties are highly uncertain due to the limited data available. Numerical exercises concerning flow patterns in the nonwelded units below the repository have shown that the portion of flow in the matrix versus the fractures varies widely depending on the assigned hydrologic parameters (Robinson et al., 1997). Key parameters used to calibrate the LBNL UZ Flow Model are the matrix saturated hydraulic conductivity (K_{sat}) and the F/M interaction reduction term for the nonwelded units.

There are three general types of nonwelded tuff below the repository, each with different flow and transport properties and, hence, different effects on flow patterns: vitric, devitrified, and zeolitic. Based on borehole data near the repository, the Calico Hills Formation, Prow Pass Tuff, and Bullfrog Tuff are composed of varying thicknesses of each type of nonwelded tuff. A complicating factor is that the three types of nonwelded tuffs lack horizontally continuity and the locations of horizontal transitions from one layer type to another are highly uncertain. For example, because zeolite formation is a secondary alteration process, the distribution of zeolitic tuffs does not follow the primary stratigraphy. The degree of welding, from nonwelded to partially welded, is also expected to impact the hydrologic properties of the tuff. Borehole logs indicate that lateral variations in the degree of welding is a feature of the Prow Pass Tuff. Unfortunately, characterization of these lateral variations in the alteration and in the degree of welding in the subunits for incorporation into UZ flow and transport models may not be possible, given the limited number of boreholes.

Another point to consider is that the layer types through which water flows en route to the water table also varies. For example, owing to the downward 5-10° slope of stratigraphic units at YM, the water table is in the Calico Hills Formation east of the repository footprint: within the repository footprint, the water table is in the Prow Pass Tuff on the eastern side and in the upper Bullfrog Tuff on the western side. The slope of major hydrostratigraphic units is explicitly considered in the LBNL UZ Flow Model.

Within boreholes, the contacts between layers and sublayers range from gradational to abrupt. Based on the stratigraphic classifications of Rautman and McKenna [1997, (table 1)], there are six subunits in the Calico Hills Formation and five in the Prow Pass Tuff. In the DOE UZ transport model (Robinson, 1997; Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998) this total of

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11 layers is modeled using only 6 model layers. Given the small-scale variations and the uncertain distribution of large-scale variations, there is little confidence that volume averaging in the site-scale LBNL UZ Flow Model accurately captures the flow field.

Sparse data are available from which to determine flow patterns in the nonwelded tuffs below the repository. Laboratory core-scale (~ 5cm) measurements of permeability include 6 measurements on vitric rock types, 3 on bedded tuffs, and 69 on zeolitic samples (Flint, 1998). For the VA, fracture characterization data from the PTn was used as an analog for the Calico Hills nonwelded units (CHn) because there were only two boreholes with pertinent fracture data that had Q-status (Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998). It is suggested that fractures may be more abundant in the PTn than in the CHn (Sweetkind et al., 1997); thus, this is apparently a conservative choice. Little data are available for characterization of fracture hydrologic properties in vitric and zeolitic layers. Water saturations and chemistry suggest the vitric units readily drain and contain younger water with lower dissolved solid concentrations compared to water in zeolitic tuffs (Bodvarsson et al., 1997).

The areal extent and volume of perched waters are unknown. An understanding of the change in hydrologic and transport properties in relation to the variation in alteration in the nonwelded units and the welding in the Prow Pass Tuff would clarify flow paths and velocities and also the magnitude of sorption in the non-welded to partially-welded units below the repository. The paucity of data has led to a reliance on numerical modeling.

Given the scarcity of data or supporting measurements, the use of a 3D flow field does not directly imply that the flow patterns below the repository are known with any certainty. The LBNL UZ Flow Model accounts for only general large-scale features in the model domain. This is especially true given that nonunique parameter sets, calibrated with emphasis on areas where abundant data were available, are assigned over the entire model area. Given the sensitivity of TSPA predictions to the fraction of flow through nonwelded layers, smaller scale models should be used to delineate flow properties through the nonwelded units below the repository. Such models would prove useful for determining (i) distribution of vertical flow in the matrix and fracture system for each unit, (ii) spatial variability of flow rates in each unit, (iii) location and magnitude of lateral flows (i.e., diversion around unfractured layers), and (iv) flow behavior across the boundary between each unit (i.e., gradational or abrupt boundaries).

In the TSPA-VA Technical Basis Document (Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998), sensitivity analyses of hydraulic properties on flow rates in the matrix and fracture system using a 1D model suggests that decreases in the permeability of zeolitically altered tuffs will not significantly impact the flow and transport pattern. Sensitivity analyses with the DKM and DKM/WEEPS models [U.S. Department of Energy, 1998 (volume 3)] confirm this. However, the properties of the vitric and devitrified subunits appear to significantly impact performance. Detailed process models for the hydrostratigraphic units and unit pairs would clarify our knowledge of the flow and transport patterns as well as create a basis for uncertainty analyses.

Robinson et al. (1997) showed the importance of including spatial heterogeneity of the units. Where vitric subunits transition into zeolitic subunits in the LBNL UZ Flow Model, the model pinches out the former and pinches in the latter. The threshold for classification of zeolitic versus vitric subunits is that subunits with more than 10 percent zeolite alteration by weight are considered zeolitic. This threshold provides no physical basis for hydrologic or sorption parameter values but it does reflect a reasonable cutoff, given the bimodal distribution of zeolite weight percent. Research by Rautman and McKenna (1997) and Carey et al. (1997) on the distribution of minerals should be supplemented more completely with hydrologic property characterizations of slightly altered vitric and devitrified tuffs, together with the variations associated with changes in the degree of welding. From a physical process basis, the permeability should decrease as the alteration increases due to a reduction in the pore sizes. Robinson et al. (1997) use porosity as a predictor of permeability in their heterogeneous model. However, porosity variation is a poor predictor for changes in permeability caused by zeolitic alteration; the difference in the means and ranges of porosity in vitric versus zeolitic tuffs is extremely small, while the differences in permeability can be quite large (Flint, 1998).

Along with variations in permeability of the nonwelded tuffs, their capacity for sorption of radionuclides also varies widely. Given that little flow through the matrix of zeolite horizons is expected (owing to low matrix permeability and fracture density), the sorption properties of the vitric and devitrified subunits are expected to have the largest influence on transport of radionuclides to the water table. In these units with little or no zeolitic alteration, flow is expected primarily in fractures where sorption of radionuclides on fracture walls is likely small due to the small mineral surface area. With respect to variation in zeolite content and sorption characterization, the nature of the distribution of small amounts (<10 wt %) of zeolite will be important. If the zeolite is localized, the small-scale flow patterns may divert around the zeolite patches or lenses. Thus, little impact on sorption due to the zeolites would be expected. If the distribution of zeolitic alteration is more uniform and matrix permeability can accommodate sufficient flow, then radionuclide sorption may provide a significant benefit to repository performance. Sorption properties of non to slightly altered vitric and devitrified tuffs are addressed under the NRCs Radionuclide Transport Key Technical Issue.

The importance of underlying model assumptions to reliable predictions of flow and transport through the matrix of nonwelded units is discussed in the TSPA-VA Technical Basis Document [U.S. Department of Energy, 1998 (chapter 7)]. Sensitivity studies on the LBNL UZ Flow Model suggested that predicted flow from vitric into zeolitic tuffs was excessive when upstream weighting[2] of the permeability and relative permeability was used (Robinson et al., 1997). This led to a significant shift (order of magnitude in time) in the breakthrough curves at the water table due to increased travel times and sorption from unlikely radionuclide movement into and through the zeolitic tuff rather than through fractures. To reduce this error, the TSPA-VA reports that downstream weighting is now used between cells of vitric overlying zeolitic. Although the change to downstream weighting is an important modification, it is still not clear what the correct flux into the zeolitically altered tuff should be. The contact between the vitric and zeolitic horizons varies from sharp to gradational with vertical transition zones of up to 70 m. Little flow into altered horizons would be expected where sharp contacts, such as for a highly fractured, welded vitric unit, overlie a zeolitically altered horizon.

In summary, a deterministic approach with uniform properties in each layer is used for flow and transport below the repository where the paucity of measurements or characterization instead suggest a heterogeneous approach implemented through a stochastic model might be more appropriate. Incorporation of work along the lines of Rautman and McKenna (1997) or Carey et al. (1997) into a transport-scale model would be extremely useful. This was done by Robinson et al. (1997) using a refined site-scale grid and the addition of a mineralogy module to include permeability and sorption variations based on variations in alteration. However, variations in permeability and K_d corresponding to zeolite content require more characterization to provide a more rigorous basis for the methods used by Robinson et al. (1997). In addition,

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[2]Upstream weighting refers to use of the permeability value assigned to the upstream cell when simulating flow from one model cell to another.

in the Robinson et al. (1997), model, it does not appear that properties of devitrified horizons or variations in the degree of welding (nonwelded to partially welded) were included.

5.1.2 The U.S. Department of Energy Unsaturated Zone Radionuclide Transport Model

For the TSPA-VA, the Site-Scale UZ Model of YM (Bodvarsson et al., 1997) is used to obtain groundwater flow vectors for both fracture and matrix continua, including flow between fracture and matrix. These flow fields are used as input to the FEHM particle tracking code, which employs a residence time transfer function (RTTF) approach to account for the effects of hydrodynamic dispersion, radionuclide sorption, and matrix diffusion. The particle tracking method used is a cell-based approach that sends particles from one model cell to adjacent cells based on residence time calculations. The RTTF is basically a cumulative distribution of relative residence times that can be defined by any number of analytical solutions of the advective-dispersive equation. Each time a particle moves into a model cell, it is assigned a residence time that is a function of both the advection velocity and a random component determined from the RTTF. This approach is described in detail by Robinson et al. (1997) and in the TSPA-VA Technical Basis Document (Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998).

The RTTF can be used to simulate solute transport using either single- or dual-permeability flow fields. The present DOE formulation employs the RTTF using dual-permeability flow fields; thus, flow in and between both fracture and matrix continua is explicitly considered. It also appears that a third continuum is implicitly considered when the RTTF is formulated using a solution to the advection-dispersion equation that accounts for matrix diffusion (e.g., Tang et al., 1981). Conceptually, this third continuum represents an immobile reservoir in contact with the fracture continuum, but not the matrix continuum. The concerns with this third continuum approach to modeling matrix diffusion were brought to the attention of DOE following the March 1998 TSPA Technical Exchange,[3] and discussed in the NRC IRSR on Unsaturated and Saturated Flow Under Isothermal Conditions (Nuclear Regulatory Commission, 1998); these concerns are repeated in section 5.1.3.

As formulated in the TSPA-VA (U.S. Department of Energy, 1998), radionuclide particles tracked through the model domain can be transported in any of the four following ways: (i) in the fracture continuum by advection and dispersion, (ii) in the matrix continuum by advection and dispersion, (iii) between the fracture and matrix by advection, and (iv) between fractures and an immobile third continuum by matrix diffusion. Colloid transport and decay of radionuclides are also included in the RTTF approach, but are not discussed here.

It is difficult to assess the magnitude of solute dispersion that occurs in the RTTF approach, especially when applied to UZ flow. The DOE uses a range of dispersion length values from 7.5 to 32.5 with an average value of 20 m. It is not clear that dispersion lengths used in the DOE particle tracking model can be related to longitudinal and transverse dispersivity used in classical solutions of the advection-dispersion equation. Dispersion in the RTTF method is assumed to be 1D axial-symmetric. Instead of using longitudinal and transverse dispersivity values relative to the principle direction of flow, a single dispersivity value is used, along with cell dimensions, to derive directional dispersivity values. This approach appears to work well with a 1D, single-permeability continuum model [e.g., Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (figure 7-4)], however, for 2D and 3D dual continuum models

[3]Letter to S. Brocum, U.S. Department of Energy, July 6, 1998.

of the RTTF, approach has not been rigorously validated. Also at issue, there is no basis for estimating dispersion length values for the UZ at YM. For saturated flow and transport problems, values of longitudinal and transverse dispersivity values are typically approximated using available literature (e.g., Gelhar et al., 1992) when there is no site-specific information. Ranges of values for longitudinal and transverse dispersivity applicable to UZ transport are not readily obtained from the literature and no site-specific values have been estimated for YM.

One of the assumptions in the RTTF method is that the system is advection dominated [Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (section 7.4.2.2)]. For highly dispersive transport, the RTTF method is operational although the amount of dispersion may not be comparable to that produced using conventional solutions to the advective-dispersive equation. Yet, the primary natural barrier for radionuclide migration in the UZ is through the nonwelded vitric, devitrified, and zeolitic tuffs where dispersion is significant and may dominate the advection component. Conventional solutions to the advective-dispersive equation are appropriate for the flux through the nonwelded units and would be useful for comparison to the RTTF results in a submodel domain.

It is also difficult to assess the magnitude of dispersion predicted by the RTTF approach over the entire model domain, considering both fracture and matrix flow and transport. For model grids not aligned with the principle direction of flow, cell-to-cell movement of radionuclides, based on pure advection, results in numerical dispersion. Given the complex flow paths below the repository, it is not possible to align model grids with the flow field. In the TSPA-VA Technical Basis Document (Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998), results from a 2D saturated zone transport problem—with grids not aligned with the flow field—are presented as demonstration that no numerical dispersion is produced by the RTTF method. From the plot of results (figure 7-8, section 7.4.3.3), it is shown that less dispersion occurs using the RTTF model than when a numerical solution of the advective-dispersive equation is used. However, this example is not proof that the RTTF method produces no numerical dispersion, as the model considers transport over a relatively short distance of about 60 m between injection and collection wells.

The RTTF method creates artificial numerical dispersion whenever the node connections are not aligned with the principle direction of flow. For example, consider a grid aligned 45 °C to the flow field, as shown in figure 5-1, where nodal connections are used rather than cell faces. A particle released at point A has a 50 percent probability of going to point B and a 50 percent probability of going to point C with the movement along the y-axis being $\pm\Delta/\sqrt{2}$, where Δ is the distance between nodal connections. The variance in position along the y-axis after one step is $(\Delta^2/2)$. After n steps (where $n >> 1$), the Central Limit Theorem implies the distribution along the y-axis should be approximately normal with a variance of $n \ (\Delta^2/2)$. By definition (Bear, 1972), the transverse dispersion is

$$D_T = \frac{\sigma_T^2 v}{2x} = \frac{(n\Delta^2/2)}{(2n\Delta/\sqrt{2})} \qquad (5\text{-}1)$$

where σ^2 is the variance, D_T is the transverse dispersion, and v is the velocity. This implies that numerical transverse dispersion is

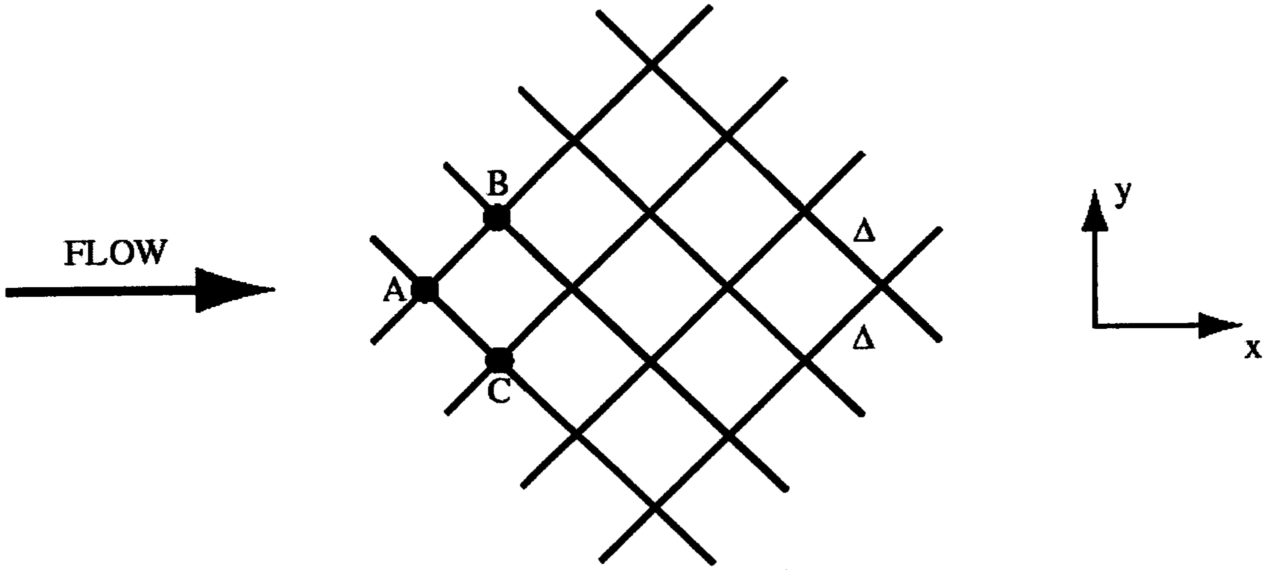

Figure 5-1. Node connections for particle transport with a mesh oriented at 45° to the direction of flow. The coordination number for each node is four and all cells are square with sides of length Δ. Numerical dispersion occurs in such a model because, for example, particles moving in the x-direction from point A are forced to pass through points B and C, causing them to spread laterally due to this unintended y-component of flow.

$$\alpha_{T\text{numerical}} = \frac{\sqrt{2}}{4}\Delta \qquad (5\text{-}2)$$

The mesh in figure 5-1 is similar to the mesh used for horizontal layers in the repository footprint. A higher coordination number may reduce dispersion, however, alignment of node connections will not always coincide with the flow field below the repository, regardless of the coordination number.

The LBNL site-scale model grid has areas where the alignment of the grid does not correspond with the principle direction of flow. The vertical gridding is structured in that the 3D grid is essentially a stacked collection of identical 2D horizontal grids. Hence, the predominance of vertical flow is in areas of vitric horizons, and the stacked grid alignment perpendicular to the direction of flow leads to a lessening of the dispersion problem locally. However, below the repository, there is both lateral and vertical flow—especially in zeolitically altered areas—where numerical dispersion could be a problem. The grid in the horizontal plane in the repository footprint is also structured, as it is aligned north-south and east-west. Lateral flow may range from northeasterly to southeasterly in this area, but is more likely to be easterly due to the easterly dipping bedding planes (typically dipping easterly at 5–10 °C). East of the repository footprint, the horizontal grid is truly unstructured and the orientation is unlikely to coincide with the flow paths. Dispersion will be created in any area where there is some component of lateral flow even without considering the horizontal grid orientation with respect to the horizontal component of the flow direction.

Conceptually, numerical dispersion may affect performance prediction because dispersive dilution leads to a reduction in the peak mass flux and increases the flux of radionuclides into nonwelded subunits, such as the zeolitic horizons, where enhanced radionuclide sorption occurs. The TSPA-VA reports that sensitivity studies for the RTTF approach indicate dispersion is not important. Likely reasons for this conclusion are the complex flow paths below the repository and the uniform release of radionuclides over a large area (repository subareas). If there is no basis for choosing a value of dispersion length, and dispersion is determined unimportant, then dispersion could readily be removed from the modeling. However, the dispersion length value will have a larger impact for more focused releases from the repository such as from individual—or groups of—WPs as is expected in the initial 10,000-yr period. The emphasis on transport modeling typically has been for time periods longer than the 10,000 yr; however, if the regulatory compliance period for performance of the repository is set at 10,000 yr, as expected, modeling efforts should have an increased emphasis on focused releases. Under a focused release scenario, the basis for selection of dispersion length values and an analysis of the numerical dispersion is more important.

5.1.3 Matrix Diffusion in the Unsaturated Zone

The term matrix diffusion refers to the diffusive exchange of dissolved constituents between water flowing in rock fractures and the essentially stagnant water that occupies the pore spaces of the rock matrix. The overall importance of matrix diffusion in the UZ depends on several factors, including

- The effective diffusion coefficient which, in turn, is a function of rock matrix saturated porosity and tortuosity, and the solute-specific free-water diffusion coefficient;
- The fracture flow system geometry (i.e., fracture spacing) that defines the size and shape of the rock matrix blocks and, hence, the matrix surface area available for diffusive exchange with fracture waters;
- The time scale for transport through the UZ (a function of fracture flow velocity and transport distance) relative to the time scale for diffusion into the rock matrix (a function of effective diffusion coefficient and flow system geometry); and
- The solute aqueous concentration gradient across the F/M interface, is affected by initial solute concentrations in the rock matrix and fractures, and also by solutes that may enter the rock matrix by means other than diffusive transport through rock matrix (e.g., via matrix-matrix and F/M advection).

Matrix diffusion is most effective as a dilution mechanism in a saturated flow system where closely-spaced fractures dissect a porous rock matrix and transport velocities are slow (or the transport path length is long). In such a system, there is a large surface area for diffusive exchange and plenty of time for the exchange to occur. For sorbing solutes, the dilution benefits of matrix diffusion are significantly enhanced because the solutes gain access to a vast increase mineral surface area available for sorption; additionally, solute sorption acts to maintain greater aqueous concentration gradients across the F/M interface.

The UZ flow system at YM provides less than optimal conditions for effective matrix diffusion for several reasons. First, the system is unsaturated: in unsaturated fractures, the wetted F/M interface area is reduced from that in a saturated system. In unsaturated rock matrix, diffusive transport is reduced as the saturated cross-sectional area is decreased and tortuosity increased. Second, the transport distances from the proposed repository to the water table are short (generally, less than 300 m).

The DOE treatment of matrix diffusion does not appear to have changed significantly from the model described by Robinson et al. (1997). The effects of matrix diffusion are included in the DOE UZ transport model by using the analytical solution of Tang et al. (1981) to generate the RTTF, as previously described in section 5.1.2. This analytical solution uses the simplifying assumption of a semi-infinite matrix continuum (i.e., solutes diffusing into matrix blocks never reach a block center). Although matrix blocks are clearly of finite size, the semi-infinite approximation is a valid approach when the time scale for advective transport through the fracture system is much shorter than the time scale for diffusive transport to the matrix block center. The validity of the semi-infinite matrix approximation is shown by DOE in section 7.4.2.3 of the TSPA-VA Technical Basis Document (Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998) by showing that the typical fracture spacing in the UZ is greater than the calculated diffusion length. As such, the authors conclude that the semi-infinite matrix approximation is reasonable for the transport characteristics of the UZ beneath the proposed repository horizon.

To analyze the effectiveness of the RTTF approach, cumulative residence-time distribution (i.e., breakthrough) curves were generated using a 1D single-permeability model for various matrix diffusion rates and sorption coefficients. Results were compared with results obtained using the 1D analytical solution of Tang et al. (1981): the two model approaches produce quite similar results [Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (figure 7-6)], indicating the effectiveness of the RTTF approach. However, it is not clear that such favorable results would be obtained from the RTTF approach if applied to a dual-permeability model.

When the matrix diffusion RTTF is used, particle residence times—in fracture cells only—are increased to account for time spent diffusing into an immobile matrix domain, however, the particles are never actually transferred into matrix cells. Hence, a third continuum is implicitly incorporated into the transport model, where particles reside for a certain time in an immobile matrix region. This concerns the authors because the combined use of a matrix diffusion RTTF and the dual-permeability formulation invalidate two key assumptions of the Tang et al. (1981) solution: (i) that solutes exchange between the matrix and fracture systems occurs by diffusion only and (ii) that no advection occurs in the matrix continuum. Conversely, in the dual-permeability approach used in the TSPA-VA, significant advection occurs within the matrix continuum, and significant advective exchange occurs between the fracture and matrix continua. For example, simulations reported in the TSPA-VA for the base case property set and long-term average infiltration show that nearly 80 percent of flow may be significantly delayed en route to the water table due to advective transport through the rock matrix [e.g., U.S. Department of Energy, 1998 (volume 3, figure 3-10)]. With such a significant fraction of solutes traveling through rock matrix, the requisite boundary conditions for the Tang et al. (1981) solution are clearly violated. In simpler terms, although diffusive transport can occur in either direction, the DOE UZ transport model favors diffusion from fractures to matrix over diffusion from matrix to fractures.

In the TSPA-VA, it is reasoned that, because the average distance between a radionuclide in matrix and the nearest fracture would be much greater than the average distance between a radionuclide in a fracture and the nearest matrix, the model bias introduced by advection in the matrix should be minimal. Of course, this assertion implies that real advective transport through the rock matrix must be evenly distributed throughout the matrix domain. Even if such were the case, it remains to be verified, perhaps using a small-scale discrete feature model, that the RTTF model bias introduced by advection in the matrix domain is indeed minimal.

In sensitivity analyses conducted for the TSPA-VA, DOE staff conclude that matrix diffusion has a minimal influence on travel times for nonsorbing radionuclides, but was found to significantly impact travel times of sorbing radionuclides. For both sorbing and nonsorbing radionuclides, the impact of matrix diffusion in these sensitivity analyses was only significant when effective diffusion coefficients were greater than 10^{-12} m^2/s. The assessment of minimal influence was based on sensitivity analyses conducted using 2D simulations with flow fields generated using the FEHM code. However, the TSPA-VA Technical Basis Document [Civilian Radioactive Waste Management System, Management & Operating Contractor, 1998 (figure 7-27)] shows results of 3D sensitivity analyses that clearly indicate significant attenuation of mass-flow to the water table for nonsorbing solutes due to matrix diffusion. The reason for the disparity between the importance of matrix diffusion in 2D versus 3D models is not clear, nor is it discussed by DOE. Given the apparent disparity between the results of the 2D and 3D sensitivity analyses, the authors find the conclusions drawn from the 2D analyses unconvincing.

For the TSPA-VA base case, the assumed matrix diffusion coefficient is 3.2×10^{-11} m^2/s for all transported radionuclides [U.S. Department of Energy, 1998 (volume 3, section 4.1.11)]. This assumed value is consistent with laboratory values measured for the relatively slow-diffusing TCO_4^- anion in saturated tuff (Triay et al., 1997). Because the same diffusion coefficient is assigned to all transported radionuclides, it is appropriately conservative that a low value be chosen. However, the use of a diffusion coefficient based on a saturated system is not appropriate for unsaturated systems because there is reduced pore volume available for diffusive transport. Thus, diffusion coefficients should be scaled as a function of saturated porosity. In addition, only a small fraction of F/M interface area is expected to be actively flowing. Thus, the effective matrix diffusion coefficient used in the UZ transport model should be further reduced using some type of F/M interface reduction factor, similar to that used in the LBNL Flow Model calibration [Bodvarsson et al., 1997 (chapter 6)].

Sensitivity of the TSPA-VA base case to matrix diffusion was evaluated by DOE [1998 (volume 3, section 5.6.1)]. Assuming base case parameter values for all other parameters, the difference in TSPA-VA predicted for dose rate (mrem/yr) was minimal; the only noticeable difference in model results was a 2,000-yr arrival time of the earliest doses with no matrix diffusion in the UZ versus a 2,400-yr arrival time for the case with matrix diffusion.

In addition to the technical concerns with the DOE approach to including matrix diffusion into the UZ RT model, there is geochemical evidence that diffusive exchange of solutes between matrix and fractures at YM may be quite limited. In a summary report of YM geochemical characteristics, Murphy and Pabalan (1994) point out significant differences between the chemical signatures of matrix pore water and fracture water in the UZs near YM and Rainier Mesa.

Given the minimal benefit of matrix diffusion to predicted repository performance, the number of technical concerns with the DOE approach, and the geochemical evidence of disequilibrium between matrix and fracture waters, the authors recommend that DOE eliminate or significantly reduce the credit taken for matrix diffusion in their UZ radionuclide transport model.

5.2 REVIEW OF ALTERNATE CONCEPTUAL MODELS

The development of a transport-scale model (i.e., below the repository to the water table) is recommended to evaluate the complex flow and transport patterns through and around the nonwelded tuffs below the repository. This could be accomplished as an extension of the heterogeneous model presented by Robinson et al. (1997) that used a refined grid below the repository. The geostatistical model used by Rautman and McKenna (1997), and the geologic interpolation and extrapolation of the variations in the nonwelded subunits by Carey et al. (1997), would be useful for assigning hydrologic properties. However, additional measurements of UZ hydrologic properties are needed. In particular, the relationships between hydraulic properties, sorption properties, the degree of alteration, and the degree of welding need to be investigated in more detail. The heterogeneity of vitric and devitrified horizons also needs further evaluation. Results of this transport scale model could be used to support the transport calculations made using the site-scale UZ model. The approach in the LBNL UZ Flow Model was to use a threshold of 10 wt % zeolite in each of four layers containing both vitric and zeolitic nonwelded tuffs. Areas with less zeolite content were modeled using the hydraulic and sorptive properties of the vitric tuffs, while areas with zeolite content greater than the threshold were modeled using zeolitic tuff properties. Evaluations of the distribution of zeolites have been conducted by Carey et al. (1997) using larger threshold values (20 wt %) and by NRC (1998) using smaller threshold values (2.5 wt %). Results of these evaluations show that the model area covered by zeolitic layers changes significantly when different threshold values are used.

Another approach, more in line with the NRC TPA model, would be to develop maps of composite thicknesses of vitric and zeolitic horizons that lie between the repository and the water table, using such data as compiled in Carey et al. (1997) and in borehole log information. For example, figure 5-2 was developed using a 10 percent zeolite threshold and inverse distance interpolation to delineate vitric from zeolitic horizons. The sharp changes between boreholes SD-12, WT-2, and SD-7 in the center of each figure may be indicative of the pattern of variation in the lateral extent of alteration. Such sharp changes in rock properties could locally impact the flow patterns. The data gap to the west and south of these three wells prevents adequate characterization of the transition between the strongly zeolitized alteration to the north Calico Hills subunits and the nonaltered vitric subunits to the south. Note that in figure 5-2, the presence of vitric and zeolitic subunits is continuous across the repository footprint.

5.3 SUMMARY OF CONCERNS

The authors agree that the overall approach in the TSPA-VA for calculating movement of radionuclides to the water table may be reasonable and appropriate. Despite the appropriateness of the overall approach, however, supporting bases are needed to gain confidence in the methodology and in the parameter ranges. There are a number of concerns that require further documentation or study:

- There is little supporting data for the hydrologic and transport parameter values used in the modeling studies of transport below the repository. Ongoing studies in the Busted Butte Transport Facility will be useful to answer some of the questions concerning matrix and fracture flow in the vitric unit. This field experiment will also contribute to characterization of permeability and sorption in a slightly altered vitric tuff. However, hydrologic and transport property variations related to extent of alteration and welding are not known. Additionally, the hydrologic properties of the nonwelded devitrified tuffs have not been adequately characterized.

- It is not clear that the LBNL UZ Flow Model properly represents the complex flow field below the repository. The uncertainty in the UZ flow patterns, acknowledged by DOE, needs to be addressed and incorporated into TSPA analyses. Again, it appears that the Busted Butte Transport Facility will address some of the uncertainty regarding flow patterns in the nonwelded units. However, larger scale vertical and lateral flow patterns in the vitric and devitrified units will remain highly uncertain.

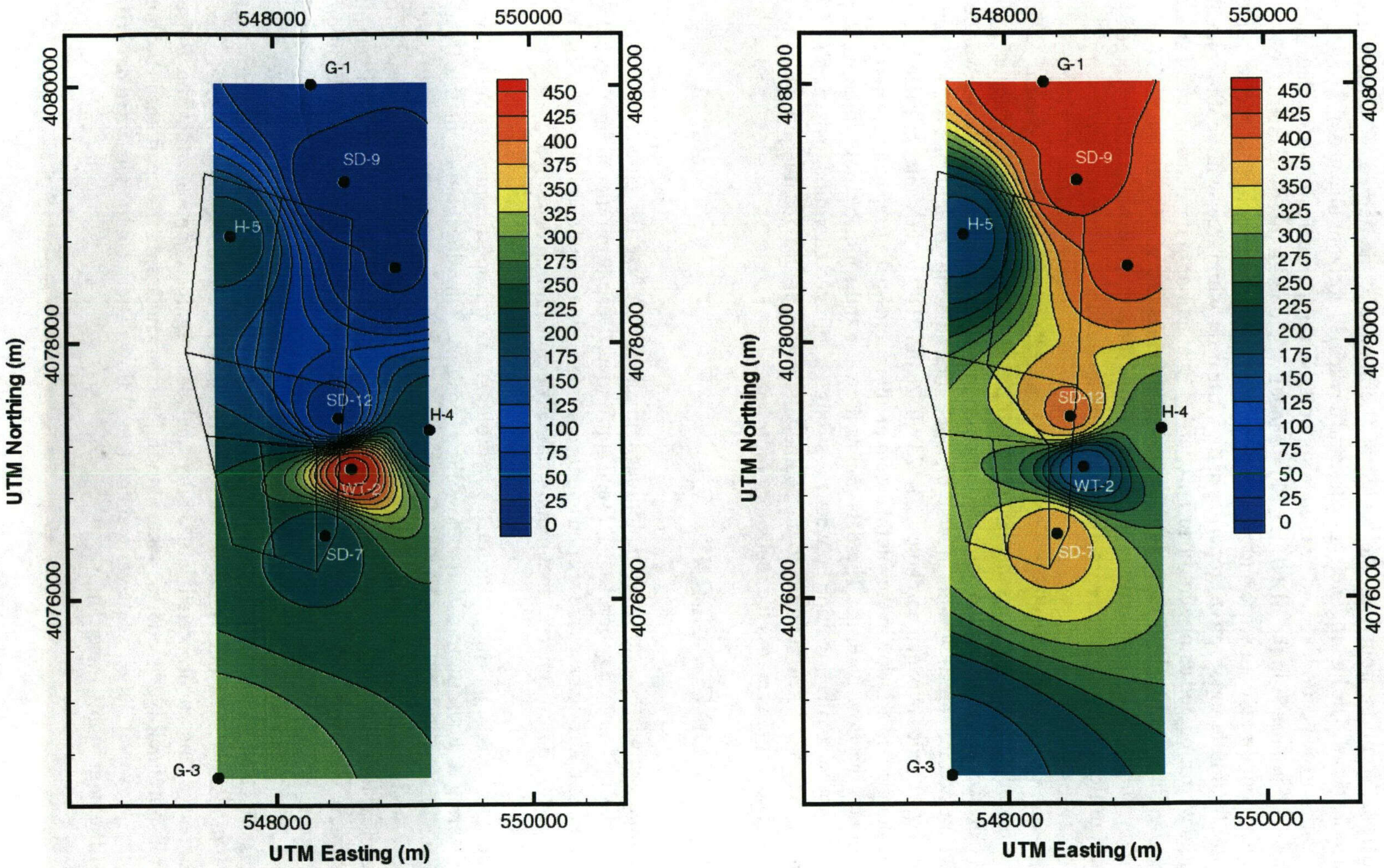

Figure 5-2. Color contour maps showing interpolated horizon thicknesses of vitric (left) and zeolitic (right) nonwelded tuffs beneath the proposed repository footprint. Thicknesses are based on stratigraphy from 9 boreholes (●) in the vicinity of the repository footprint, assuming a classification threshold of 10 percent zeolites by weight.

- Validation of the RTTF method is needed before results can be accepted with reasonable confidence. The method is ideal for advection dominated transport through the fracture continua, but flow and transport through the matrix of nonwelded units are considered the primary natural barrier in the UZ below the repository. The issue of artificial numerical dispersion in the RTTF model will become more important as focused releases over the first 10,000-yr period are given increased emphasis in PA.

- The consequences of decoupling matrix diffusion from matrix advection in the RTTF approach are not well understood and may result in overestimation of matrix retention processes.

5.4 PATHS TO RESOLUTION

The concerns in the previous section can be addressed through the following paths:

- The flow fields through the predominantly nonwelded units remain highly uncertain, which as a result, so does the magnitude of sorption and timing of arrival to the water table. Field experiments in the nonwelded units below the repository must be used to support the conceptualization of the flow fields represented by the simulated models. Further work at the Busted Butte Transport Facility on flow patterns near highly zeolitized tuffs would be useful, presuming there are zeolite horizons immediately below the facility[4]. The extent of matrix and fracture flow at various percolation rates in the vitric and devitrified horizons requires additional work in the area of F/M interaction coefficient.

- A transport scale model incorporating heterogeneity should be developed and compared with the results of the site-scale flow and transport simulations. For the transport scale model, the variation in hydrologic and sorption properties corresponding with variations in alteration and degree of welding should be characterized for the Calico Hills Formation and Prow Pass and Bullfrog Tuffs.

- Validation of the RTTF model, both with respect to numerical dispersion and for transport in the matrix of nonwelded units, is required to gain confidence that too high a proportion of radionuclides do not move through nor are sorbed in the matrix of nonwelded units. There is a need to look at other approaches to both bound the effects and support the RTTF approach. Conventional particle tracking could be implemented so that dispersion can be incorporated in a more defensible manner. This would necessarily include an interpolation of the velocity fields from the unstructured grid used by LBNL to any point in the 3D domain; although tractable, this would not be straightforward. Solution of the advection-dispersion equation directly is recommended in the vicinity of the nonwelded units where the significance of dispersion relative to advection becomes more important.

- If credit is to be taken for UZ matrix diffusion in TSPA calculations, detailed small-scale discrete feature models are needed to verify that the RTTF approach can provide a reasonable approximation of matrix diffusion effects when used with the dual-permeability formulation. Additionally, the assumed value of the diffusion coefficient for radionuclide diffusion must be appropriately scaled to account for diminished diffusive transport due to reduced matrix saturation and reduced F/M interface area in the UZ.

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[4]Giles Bussod, Los Alamos National Laboratories, to R. Fedors.

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