WBS: 1.2.5.4
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Civilian Radioactive Waste Management System
Management & Operating Contractor

Chapter 2
Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document

Unsaturated Zone Hydrology Model

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August 14, 1998

Prepared for:

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

Prepared by:

TRW Environmental Safety Systems Inc.
1261 Town Center Drive
Las Vegas, Nevada 89134

— Part 1

Under Contract Number
DE-AC08-91RW00134

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Unsaturated Zone Hydrology Model

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FIGURES

TABLES

ACRONYMS

BF	Bullfrog unit
CDF	cumulative distribution function
CHnv	Calico Hill nonwelded vitric unit
CHnz	Calico Hill nonwelded zeolitic unit
CH1vc	Calico Hills vitric unit
CH1zc	Calico Hills zeolitic unit
CRWMS	Civilian Radioactive Waste Management System
DKM	Dual Permeability Model
DLS	Detailed Line Survey
DST	drift-scale test
DTN	data tracking number
ECM	Equivalent Continuum Model
ESF	Exploratory Studies Facility
FEP	features, events, and processes
FY	fiscal year
GECM	generalized equivalent continuum model
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LTA	long-term average
MAP	mean annual precipitation
M&O	management and operating contractor
Mm	matrix m
PA	performance assessment

PAPR	Performance Assessment Peer Review
PDF	probability density function
PPw	Prow Pass welded unit
PTn	Paintbrush Tuff nonwelded unit
QA	quality assurance (Q refers to qualified work; NQ refers to nonqualified work)
SHT	single-heater test
SNL	Sandia National Laboratories
SZ	saturated zone
TCw	Tiva Canyon welded unit
TDIF	Technical Data Information Form
TH	thermal hydrology
TSw	Topopah Spring welded unit
TSPA-VA	Total Systems Performance Assessment for the Viability Assessment
TSPA-LA	Total Systems Performance Assessment for the License Application
USGS	United States Geological Survey
UZ	unsaturated zone
UZFEE	Unsaturated-Zone-Flow Expert Elicitation
YMP	Yucca Mountain Project

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2. UNSATURATED ZONE HYDROLOGY MODEL

2.1 INTRODUCTION

The - (UZ) flow analysis of Yucca Mountain comprises four sub-components (climate, infiltration, mountain-scale UZ flow, and seepage into drifts) that are believed to play an important role in the performance of the potential repository. Climate and infiltration influence the amount of water percolating toward the repository. Subsequently, water seeping into the drift and onto the waste packages can accelerate waste-package degradation, and rapid pathways from the repository to the water table via fractures can decrease the transit time of radionuclides to the accessible environment. Prediction of these events relies on process models of UZ flow that have been tested or calibrated against available data at Yucca Mountain. This chapter describes the development of these models and the important processes and relevant parameters used in the Total System Performance Assessment-Viability Assessment (TSPA-VA). The assumptions, issues, and implementation of the UZ-flow models used in TSPA-VA calculations are also provided in this section.

2.1.1 Ties to Other Components

UZ flow is closely related to other model components within TSPA-VA, including UZ thermal hydrology (TH), UZ radionuclide transport, near-field, and saturated-zone (SZ) flow and transport.

- *UZ Thermal Hydrology*—Simulated UZ flow fields serve as initial conditions and, in some cases, far-field boundary conditions for TH simulations. Also, the stratigraphy and calibrated hydrologic parameters defined for UZ flow are provided to TH modelers for use in their simulations. In reverse, the results of the TH calculations are used to assess the impact of the thermal perturbation on ambient UZ flow. Mountain-scale and drift-scale TH calculations are also used to determine how to modify seepage into drifts during the thermal period.

- *UZ Radionuclide Transport*—Simulations of UZ flow fields provide the required advective component of far-field radionuclide transport. In TSPA-VA calculations, radionuclide transport is calculated using a particle-tracking transport model with the UZ flow fields as input.

- *Near-Field Geochemical Environment, Waste-Package and Drip-Shield Degradation, Waste-Form and Cladding Degradation, and* Engineered-*Barrier System (EBS) Transport*—Water seepage into emplacement drifts is a key input to all of these TSPA components. The UZ flow information that is provided to the near-field is (1) the fraction of waste packages that are subjected to seeps and (2) the distribution of seepage rates.

- *SZ Flow and Transport*—The SZ-flow model defines the bottom boundary condition for the UZ-flow model, which consists of the water-table height as a function of discrete time intervals, as defined by present-day, long-term average (LTA), and superpluvial climates.

Percolation rates at the water table are passed from the UZ-flow model to the SZ flow and transport model.

Figures 2-1 through 2-4 illustrate the ties between UZ flow and other TSPA-VA components, along with the bases for each of the four UZ-flow subcomponents (climate, infiltration, mountain-scale UZ flow, and seepage into drifts).

2.1.2 Previous Treatment in Yucca Mountain Project Performance Assessment (YMP PA) Modeling Efforts

UZ flow has been modeled extensively and with several different technical considerations in past Yucca Mountain TSPAs. The majority of the TSPA work has been based on the composite-porosity, or equivalent-continuum, flow model. TSPA-1991 (Barnard et al. 1992, pp. 4:31 through 4:53) and TSPA-1993 (Wilson et al. 1994, Chapter 8, pp. 1-17) also used an alternative conceptual model called the Weeps model, and TSPA-1995 (CRWMS M&O 1995, pp. ES-15 through ES-16, pp. 7.1-7.10) used an extension of the equivalent-continuum model dubbed the generalized equivalent-continuum model (GECM). The use of these models in the TSPAs has ranged from direct inclusion of flow codes in the TSPA calculations to abstraction of information (e.g., response surfaces) from more detailed flow codes prior to TSPA calculations.

TSPA calculations of UZ flow have previously been restricted to only one spatial dimension (i.e., assuming strictly vertical flow). TSPA-1995 (CRWMS M&O 1995) included some evaluation of the one-dimensional assumption by comparison with a two-dimensional cross section taken out of the Lawrence Berkeley National Laboratory (LBNL) three-dimensional model (Wittwer et al. 1995, pp. 13-34). They found that the one-dimensional and two-dimensional calculations compared favorably, but it is important to note that the LBNL model did not yet include adjustments for perched water at that time. The current LBNL model (Bodvarsson et al. 1997) indicates significant nonvertical flow below the repository.

In past TSPAs, two approaches have been used for modeling seepage. The most commonly used method is based on the equivalent continuum model (ECM) and assumes that the saturated hydraulic conductivity of the matrix, K_{sm}, represents a threshold for fracture flow. In TSPA-1995, for example, K_{sm} and the percolation flux q were both assumed to be (independently) distributed log-normally in space. The fraction of locations where q exceeded K_{sm} was calculated and assumed to be equal to the fraction of waste packages contacted by seeps. The amount of seepage contacting a waste package was taken to be $q–K_{sm}$ times an area that was arbitrarily chosen to be four times the physical waste-package cross-sectional area.

The second method that has been used for modeling seepage in past TSPAs is the Weeps model. This probabilistic method assumes all water flow to be in discrete fracture channels and calculates the number of those channels based on assumed distributions for fracture hydraulic properties. Any fracture flow that intercepts an emplacement drift is assumed to flow into the drift (no threshold). The number of waste packages contacted by seeps is calculated probabilistically based on the number and size of flow channels and the cross-sectional area of the waste packages. In this approach, the amount of seepage contacting waste packages is given by the hydraulic properties of the fracture channels that contact waste packages.

One of the key uncertainties in UZ flow simulations has been in the upper boundary condition; specifically, the appropriate value for the mean percolation flux and its spatial and temporal variability. It is important to note that estimates of mean surface infiltration above the repository area have increased significantly in the last 2 years (CRWMS M&O 1998, *Yucca Mountain Site Description*, Section 5.3.4.1), so the infiltration values used for TSPA-VA are much higher than those used for TSPA-1993 (Wilson et al. 1994, Chapter 8, pp. 1-17; Andrews et al. 1994, Chapter 3, pp. 1-5, 8-16, Chapter 4, pp. 6-8) and TSPA-1995 (CRWMS M&O 1995, ES-15 through ES-16, 7.10 through 7.10). The predictions of increased infiltration rates have resulted, in part, from the ability of recent models to account for explicit fracture flow in dis-equilibrium with the matrix, which results in the ability to sustain higher infiltration rates without saturating the matrix. In addition, recent models of infiltration described in Section 2.4.2 have resulted in estimates of infiltration that are higher than those of past TSPAs. These models derived infiltration estimates from precipitation data, evapotranspiration, and other surface mechanisms that are relevant to infiltration.

Past TSPAs have taken percolation to be spatially uniform, but temporal variability was included in TSPA-1993 and TSPA-1995. The temporal variability was idealized as a step function by Wilson et al. (1994, Chapter 8, pp. 1-17) and as a triangular function by CRWMS M&O (1995, ES-15 through ES-16, 7.1 through 7.10) with a period of 100,000 years (simulations were carried out to 1,000,000 years). Short-term variability in the infiltration was not considered. In TSPA-1993 and TSPA-1995, water-table rises were assumed to have the same functional form as the percolation changes (i.e., either a step function or a triangular function with a period of 100,000 years). In addition, past TSPAs have modeled flow only from the repository down, so the model boundary condition has been percolation flux at the repository, not infiltration rate at the surface.

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

2.1.3 Synopsis of Current Treatment and Changes from Prior Efforts

A primary difference in the treatment of UZ flow between TSPA-VA and previous TSPAs is the use of a fully three-dimensional UZ flow model developed at LBNL by Bodvarsson et al. (1997, pp. 2.2 through 2.15). Their goal was to synthesize all of the available data into a coherent, predictive model of water and air flow in the UZ using the dual-permeability continuum formulation of fracture and matrix flow and interaction. The numerical formulation of the model is implemented with the TOUGH2 computer code (Pruess 1991, pp. 1-4). Model calibration is performed using an inverse method implemented in ITOUGH2 (Finsterle 1993, pp. 1-23) to optimize the model parameters against available data. A new feature of the current LBNL model (Bodvarsson et al. 1997) is that a fracture-matrix coupling parameter, related to the wetted contact area between fractures and matrix, can be used as an inversion parameter in each hydrogeologic unit. The use of the three-dimensional UZ flow model precludes the need for simplified or abstracted flow fields, as has been required in previous TSPAs. However, because of the size and computational requirements of the three-dimensional UZ flow model, the emphasis in TSPA-VA has been on using selected conceptual models and parameter sets that span the range of uncertainty in UZ flow modeling, rather than randomly sampling large combinations of parameters.

Because it has become obvious that seepage is a critical contributor to repository performance, considerably more effort has been put into modeling it for TSPA-VA than in past TSPAs. The PA group has adopted a more process-based method for estimating the amount of seepage onto waste packages, using the dual-permeability flow model and a geostatistical description of the fracture heterogeneity. A number of simulations of flow around an open drift were made, with varying percolation boundary conditions, fracture hydrologic properties, and heterogeneity structures. These results were then used to develop distributions of seepage fraction (the fraction of waste packages contacted by seeps) and seep flow rate (the rate of water flow onto a single waste package) as functions of percolation flux.

As mentioned above, it is important to note that spatially variable infiltration at the surface in the current model is considerably higher than values that were being used just 2 years ago. The higher infiltrations come from the latest project infiltration model (CRWMS M&O 1998, *Yucca Mountain Site Description*, Section 5.3.4.1), which is based primarily on neutron-hole data. Infiltration is not allowed to vary in the ITOUGH2 inversions, but infiltration uncertainty is explored to some extent by performing multiple inversions, with the infiltration map multiplied by different factors. The increase in infiltration estimates has important implications for repository performance.

2.1.4 Expert Elicitation and Peer Review Panel

The YMP conducted a UZ Flow Model Expert Elicitation (UZFMEE), in which project data and models were presented to a group of experts (mostly from outside the project) so that they could provide an evaluation of the work being done (CRWMS M&O 1997). Particular emphasis was placed on estimates of surface infiltration, deep percolation, and the uncertainties associated with each. Each expert estimated probability density functions (PDFs) of infiltration. The mean values of their estimated net infiltration ranged from 3.9 mm/yr to 12.7 mm/yr, and the mean values of their estimated percolation flux at the repository horizon ranged from 3.9 mm/yr to 21.1 mm/yr. These values are commensurate with the simulated average present-day infiltration over the modeled repository (~8 mm/yr) and the simulated average percolation fluxes within the six prescribed repository subregions for the present-day base case (3.9 mm/yr to 11 mm/yr) of TSPA-VA (see Section 2.4.2.7 and Table 2-61).

Additional topics that were covered during the UZFMEE included spatial variability of net infiltration and percolation flux, temporal variability of infiltration and percolation flux, lateral diversion above the repository, partitioning of fracture and matrix flow, seepage into drifts, modeling issues, and additional data and work requirements. The experts generally agreed that the infiltration map that was used in TSPA-VA captures the general spatial variability of infiltration, but several suggested that more infiltration could occur beneath washes with thin alluvial cover. The experts also agreed that temporal behavior of net infiltration was characterized by episodic events associated with major storm events, but that most of the transient flux was attenuated within the system. With regard to lateral diversion above the repository, most of the experts agreed that contrasts in the hydrologic properties between units would likely cause lateral flow, particularly in the Tiva Canyon welded unit (TCw)-Paintbrush Tuff nonwelded unit (PTn) contact, but that the amount of diversion was limited to scales of several meters to tens of meters. This is consistent with the results of the TSPA-VA UZ-flow simulations, which show nearly vertical flow above the repository (Section 2.5.1). The experts did not address the issue of lateral diversion caused by perched water below the repository. The experts also estimated that, based on the low matrix permeabilities in the Topopay Spring welded unit (TSw), the partitioning of flow in the TSw was predominantly in the fractures. Also, the fast-flow component likely represents only a small part of the total flux. This is consistent with simulated results in TSPA-VA. With regard to seepage into drifts, the experts agreed that a capillary barrier will exist around the drifts, diverting a majority of the water around the area of the drifts. This behavior is also consistent with the TSPA-VA simulations for seepage (Section 2.4.4). Finally, the experts recommended a number of additional modeling and data-collection activities that addressed estimates of infiltration, percolation, and seepage. Many of these recommendations are included in Section 2.7.

In addition to the Expert Elicitation, a TSPA-VA Peer Review Panel provided input to the UZ flow activities. They recognized the use of environmental tracers (^{36}Cl) as evidence of fast flow paths between the surface and the repository and recommended its use in supporting the conceptual models of UZ flow. The existence of fast flow paths via fractures has been addressed through the use of the dual-permeability model, and transport times between the surface and repository are addressed in sensitivity analyses in Section 2.6.1.2.1. Although the continuum models used in TSPA-VA do not replicate the highly localized observations of bomb pulse in the Exploratory Studies Facility (ESF), travel times on the order of 50 years or less between the surface and the repository horizon are predicted in faulted regions and in models using the dual permeability model (DKM)/Weeps conceptualization (see Section 2.6.1.2.1). The Peer Review Panel also recommended studies to better understand fracture-matrix interaction, and this is also recommend in Section 2.7.3.2. Finally, the Peer Review Panel emphasized the need to better understand seepage into drifts. The method that was used in TSPA-VA is detailed in Section 2.4.4, and recommendations for future work are given in Section 2.7.4.2.

2.1.5 Objectives, Scope, and Overview of Chapter 2

The objective of this chapter is to describe the conceptual models, important issues, abstraction and implementation methods, and results of the UZ-flow component in TSPA-VA. The four subcomponents of UZ flow that will be covered include (1) climate, (2) infiltration, (3) mountain-scale UZ flow, and (4) seepage into drifts. Section 2.2 describes the processes and conceptual models associated with the four subcomponents, and Section 2.3 summarizes issues and abstraction/testing plans that were developed at the UZ Flow Workshop held December 11–13, 1996, in Albuquerque, NM. The abstraction/testing plans provided the basis for the implementation of climate, infiltration, UZ flow, and seepage models in TSPA-VA. These models and their bases are described in Section 2.4, and the results of the base-case UZ-flow and seepage models used in TSPA-VA are presented in Section 2.5. Section 2.6 describes the sensitivity analyses complementing the base-case simulations, and Section 2.7 provides a summary of the results, their implications to performance, and guidance for licensing.

2.1.6 Quality Assurance (QA) Status of Data and Simulations

A summary of the data tracking numbers (DTNs) for the relevant data and simulations used in this chapter is provided in Table 2-1 and Table 2-2. Table 2-1 lists the *source data* that were used to develop the UZ-flow models used in TSPA-VA. Table 2-2 lists the data and files that were *developed* in the UZ-flow component (the data and information contained in Table 2-2 are used by other components in TSPA-VA). Finally, Table 2-3 provides a summary of the software codes, input and output files, and DTNs associated with technical figures produced in this chapter. If the codes listed in Table 2-3 do not have a version number, then either the version number was not applicable (e.g., for small post-processors) or a software configuration management system was not implemented for the code at the institution (identified in parentheses in Table 2-3) that ran the code. In addition, unless otherwise noted, the codes used in this chapter are not yet qualified to the CRWMS M&O SI Series software procedures. Finally, because of concurrent Corrective Action Reports that pertain to the Q-status of data and software in this chapter, the status of data and software in Table 2-1 through Table 2-3 may change after the date of publication.

2.2 PROCESSES AND CONCEPTUAL MODELS

Important processes associated with each of the four major subcomponents of UZ flow are illustrated in Figure 2-5. Details of the conceptual models and processes for each subcomponent are provided in the following sections.

2.2.1 Climate

"Climate" refers to the meteorological conditions that characteristically prevail in a particular region. For TSPA-VA, climate conditions at Yucca Mountain must be known to determine the hydrology within and around Yucca Mountain. In particular, the amount of precipitation largely determines the amount of infiltration.

The climate in the Yucca Mountain region is presently warm and arid to semiarid, with mean annual temperatures of 16°C and mean annual precipitation (MAP) of about 170 mm/yr (CRWMS M&O 1998, *Yucca Mountain Site Description*, Table 4.1-12). Climate proxies, or the physical remains of substances that carry the imprint of past climates, indicate that the climate in the Yucca Mountain region is not static. For example, climate proxies indicate that during the last glacial period, between 35,000 and 10,000 years ago, most of the world was drier, but the southwest United States was wetter. At that time, the Yucca Mountain region contained wetlands and streams; there were springs at the mouth of Crater Flat and in the Amargosa Desert; there was a lake in Death Valley (Lake Manley) that was over 50-m deep; and sufficient vegetation existed to support a variety of herbivores ranging from mammoths to sheep (CRWMS M&O 1998, *Yucca Mountain Site Description*, Section 4.2).

Future climate is estimated based on what is known about past climate, with consideration given to climate impacts caused by human activities. Calcite in Devils Hole, a fissure in the ground approximately 40 km southeast of Yucca Mountain, provides the best-dated record of climate change over the past 500,000 years. The record shows continual variation, often with very rapid jumps, between cold glacial climates (for the Great Basin, these are called pluvial periods) and warm, interglacial climates similar to the present. The fluctuations average about 100,000 years in length. Because this basic time scale has been corroborated by other climate proxies (for example, oxygen-isotope variations in marine sediments), it has been selected as the average climate cycle (CRWMS M&O 1998, *Yucca Mountain Site Description*, Section 4.2.3).

Climate conditions specific to the Yucca Mountain region over this period were estimated from other, more local, climate proxies. Packrat middens are deposits consisting of plant macrofossils cemented by packrat urine that can be dated by radiocarbon methods. Plant life during the last pluvial period has been reconstructed by analyzing packrat middens. This reconstruction shows an open juniper forest in the lower elevations and a montane conifer forest in the higher elevations of the Yucca Mountain region. From modern locations with open juniper forests, it can be inferred that temperature was then approximately 6°C colder, and precipitation was approximately two times greater than modern averages (CRWMS M&O 1998, *Yucca Mountain Site Description*, Section 4.2.4.1). From global climate proxies like the Devils Hole record, the last glacial or pluvial period appears to be a rather typical climate, approaching a LTA climate in the Yucca Mountain region.

Climate proxies indicate that the last glacial period was not the most extreme climate in the record. The previous glacial period, occurring approximately 150,000 years ago, and a glacial period occurring approximately 600,000 years ago, appear to have been markedly colder and wetter. These extreme glacial climates are referred to as superpluvials. During the next-to-last glacial period, Lake Manley in Death Valley reached a depth of over 120 m (CRWMS M&O 1998, *Yucca Mountain Site Description*, Section 4.2.3.2). Lake sediments deposited by Owens Lake, north of Death Valley, hold ostracod and diatom remains of species that now live in Canada. Other evidence suggests that the vegetation in the region was mainly a dense juniper forest. This evidence supports the inference (with somewhat less confidence than inferences for the most recent glacial period) that temperature was approximately 10°C colder, and precipitation was approximately three times greater than modern averages (CRWMS M&O 1998, *Yucca Mountain Site Description*, Section 4.2.4).

The wetter environments of the past suggest that more groundwater flowed beneath Yucca Mountain. Several lines of evidence indicate that the water table was 80 to 120 m higher during the last pluvial period. The first indication is the presence of spring deposits at the mouth of Crater Flat that have been dated to approximately 13,000 years ago. In addition, a strontium-isotope ratio characteristic of the saturated zone (SZ) has been found in pore waters of rocks over 80 m above the present water table at Yucca Mountain, and carbon-isotope differences have been found as well. Lastly, water-table rises in this range have been obtained in saturated-zone groundwater modeling of future climates (CRWMS M&O 1998 *Yucca Mountain Site Description,* Sections 5.2.6 and 5.2.7). Note that the repository is planned to be over 300 m above the present water table, so the repository would still be well above the water table even with a rise of 120 m.

2.2.2 Infiltration

The conceptual model used in infiltration studies defines the physical processes determining infiltration and net infiltration, and is based on evidence provided from field studies at Yucca Mountain combined with established concepts in soil physics and hydrology (Campbell 1985, Chapter 8, pp. 73-97; Freeze and Cherry 1979; Horton 1933; Hillel 1980, pp. 109-146; Flint et al. 1996). The overall framework of the conceptual model is provided by the hydrologic cycle, which includes all the processes on the surface and in the shallow subsurface (0 to 6 m beneath the ground surface) that affect net infiltration. These processes include precipitation, infiltration, run-off and run-on, evapotranspiration, and the redistribution of moisture in the shallow subsurface. Precipitation is the dominant hydrologic process at the site because it is the source of all moisture for the surface and shallow subsurface (there are no permanent streams or bodies of surface water affecting the site), excluding water introduced to the site by human activity (dust-control, drilling, waste-water). Precipitation is dependent mostly on meteorological factors, but geographic location, elevation, and physiography are also important. Evapotranspiration is the second most dominant hydrologic process (in terms of the total volume of water involved) at Yucca Mountain and is dependent on vegetation, the distribution of available moisture stored in the shallow subsurface, and potential evapotranspiration, which is determined by an energy balance. Redistribution of moisture in the shallow subsurface occurs in response to gravity and matric potentials and is strongly dependent on soil and bedrock properties. The removal of water through evapotranspiration is dynamically integrated with the redistribution of moisture in the shallow subsurface. The generation of run-off is dependent on a combination of soil depth, soil porosity, soil permeability, bedrock permeability, and ground-surface slope. Run-on and the routing of surface flow are dependent mostly on surficial material properties, topography, and channel geometry.

The conceptual model of net infiltration has been developed from analysis of an 11-year record of neutron logs from 99 boreholes on Yucca Mountain (Flint and Flint 1995). Relative changes in water content profiles were compared against precipitation records and estimates of evapotranspiration (Hevesi et al. 1994, pp. 2323-2332). The measured changes in water content were also compared to physiographic setting, bedrock geology, and soil cover (CRWMS M&O 1998, *Yucca Mountain Site Description,* Section 5.3.4.1). In general, field studies indicated that saturated soils are established primarily during the winter in response to a series of medium to large storm events which tend to occur more frequently during periods associated with an active El Niño Southern Oscillation. The timing, intensity, and duration of precipitation, the storage capacity of the soil, and evapotranspiration determine the availability of water for net infiltration. In the upland areas of Yucca Mountain where the soil cover is shallow, the lower the effective conductivity of the underlying bedrock, the longer moisture from precipitation is held in the soil profile where it is potentially available for evapotranspiration. During winter, when potential evapotranspiration is at a minimum, smaller amounts of precipitation are needed for developing and maintaining saturated conditions at the soil-bedrock contact. When the storage capacity of the soil and the effective conductivity of the underlying bedrock are exceeded, or when precipitation intensity exceeds the infiltration capacity of the soil, runoff is generated and water is available for routing down slopes and into channels. The significance of net infiltration beneath channels in washes relative to sideslopes and ridgetops depends on the frequency and magnitude of runoff events.

Using the conceptual model, net infiltration at Yucca Mountain is characterized as an episodic, transient process depending primarily on the length of time saturated or near-saturated conditions are maintained at the soil-bedrock interface, or at a depth of 6 m in deep alluvium, and the effective conductivity of the underlying bedrock or alluvium. Net infiltration is determined as the rate of water percolation into bedrock or below a depth of 6 m in alluvium, and is limited by the effective permeability of the bedrock or alluvium. Evapotranspiration is assumed to be negligible in bedrock or below a depth of 6 m because no evidence of plant roots have been found beyond a 5 m depth. The potential for saturating the soil-bedrock interface is determined by the timing, frequency, and intensity of precipitation; the depth, field capacity, and porosity of the soil cover; potential evapotranspiration, actual evapotranspiration (which is a function of the available moisture in the soil profile), and the lateral re-distribution of surface water. Lateral redistribution of soil moisture is assumed to be negligible because the moisture-retention potential in the soil to divert flow laterally is relatively small. A detailed description of the actual determination of net infiltration is given in Section 2.4.2 of this chapter and in Flint et al. (1996).

2.2.3 Unsaturated Zone Flow

Current understanding of UZ flow in Yucca Mountain is a product of over 10 years of field observations, laboratory experiments, and numerical modeling. The most important data come from several surface-based drill holes and from the ESF, which is an 8-km-long tunnel through Yucca Mountain. Considerable amounts of data are available on rock-matrix saturations, water potentials, and temperatures; on chemical composition and isotopic abundances of groundwater and mineral deposits; on air permeability and air-pressure fluctuations; on rock types and mineralogy; on fault locations and offsets; on fracture density and orientations; and on matrix permeability and saturation/desaturation parameters (see Table 2-1). In addition, there is information on the upper boundary condition (i.e., infiltration) from a series of weather stations and shallow drill holes instrumented with neutron probes, and there is information on climatic effects from a variety of paleoclimate studies and from analogues such as present-day Rainier Mesa (see Section 2.4.2). More detailed information on conceptual models and processes involving faults, perched water, zeolites, and geothermal gradient can be found in Chapter 2 of Bodvarsson et al. (1997, pp. 2.1 through 2.15). Additional information on the site hydrogeology of the UZ at Yucca Mountain can also be found in Section 5.3.4 in CRWMS M&O (1998, *Yucca Mountain Site Description*).

Several conceptual models of unsaturated-zone flow at Yucca Mountain have been considered for TSPA-VA. Figure 2-6 illustrates the various conceptual models available to model flow through fractured media. Past TSPAs have focused on the use of ECMs. The strength of the ECM is that it can describe observed matrix saturations at Yucca Mountain. Two problems with ECM are (1) the forced-pressure equilibrium causes capillarity of the small pores to overwhelm gravity-driven flow in the fractures, leading to inaccurate descriptions of disequilibrium situations; and (2) it is computationally inefficient in solving time-variable flows. The GECM is very similar to the ECM except that a matrix satiation value less than one is prescribed to increase flow through the fractures. The GECM solves the first problem to some extent, but it suffers from lack of data to define the fracture-flow threshold and it is not clear whether it is valid under hydrothermal conditions.

The Weeps model, used in TSPA-93 (Wilson et al. 1994, Chapter 15, pp. 66-70) is a simplified stochastic discrete fracture model that only considers flow through fractures (similar to the discrete fracture conceptual model shown in Figure 2-6). It apparently predicted the fast paths observed in the exploratory-studies facility (as indicated by elevated $^{36}Cl/Cl$ occurrences) and can describe observed flow-channel spacing at Rainier Mesa (CRWMS M&O 1996, Chapter 6).

Two problems with the Weeps model are (1) it ignores the rock matrix and thus any potential performance impact of flow in the matrix; and (2) much of the data that it requires have not been collected and might be difficult (or even impossible) to collect. This model was not used in TSPA-VA because investigators favored a process-based model that could be calibrated to available site data such as borehole data and perched water.

Another important flow conceptualization is the DKM. The DKM allows computation of flow in pressure disequilibrium in matrix and fracture continua, and it appears to be a reasonable compromise between the ECM and Weeps models. The DKM conceptual model has the flexibility to represent almost the entire range of possible flow behavior through variation of the fracture-matrix coupling parameter (described in detail in Section 2.4.3.3), allowing its behavior to change continuously from the ECM (which is dominated by matrix flow) to a Weeps-type flow almost entirely within the fracture network. Because of its flexibility and ability to model a broader range of unsaturated flow problems (Ho et al. 1995, Chapter 7, p. 5; Eaton et al. 1996), the DKM conceptual model has been used in TSPA-VA. However, the DKM has its own problems, including (1) less computational efficiency than the ECM and (2) lack of data describing the coupling term between matrix and fractures.

In addition to the conceptual model for fracture-matrix partitioning, the TSPA-VA conceptual model of flow in the UZ at Yucca Mountain includes an extensive perched water zone located between the repository horizon and the water table. The perched water exists because of a low permeability region that diverts flow laterally around the perched water region (Section 2.4.3.4). Faults are also incorporated into the conceptual model of unsaturated flow and are believed to be pathways of fast flow from the surface down to the water table, giving rise to observed "bomb pulse" near faults in the ESF (Section 2.6.1.2.1).

The dual-permeability conceptual model has been used in conjunction with numerous site data to develop the UZ flow models presented in this chapter. Calibrations of the model to site data (e.g., matrix saturations, pneumatic data, and moisture potentials) and field tests (e.g., niche seepage test) have been performed to ensure consistency with observable data. However, it is important to emphasize that, while data exist to calibrate the models for UZ flow, there are not enough data to eliminate all uncertainty. One of the functions of performance assessment (PA) is to consider such uncertainties and demonstrate their relation to repository performance through the evaluation of multiple conceptual models and parameter sets. These uncertainties and alternative models are considered in Sections 2.3, 2.4, and 2.6.

2.2.4 Seepage

Seepage is the movement of liquid water into emplacement drifts. The basic conceptual model for seepage is that openings in unsaturated media act as capillary barriers and divert water around them. This capillary-barrier effect has been tested in the ESF by niche tests, in which water is injected above a niche (a side tunnel off the main tunnel). Results from the tests indicate that most of the water does not seep into an opening just two feet below. In addition, no natural seeps into the ESF tunnel have been observed, although the lack of seeps may be caused partially by drying from tunnel ventilation.

For seepage to occur in the conceptual model, the rock pores at the drift wall must be locally saturated and there must be no pore tension. Drift walls can become locally saturated by either disturbance to the flow field caused by the drift opening, or variability in the permeability field that creates channelized flow and local ponding. Of the two reasons, the variability effect is more important. Drift-scale flow calculations made with uniform hydrologic properties suggest that seepage will not occur at expected percolation fluxes. However, calculations that include permeability variations do predict seepage, with the amount depending on the hydrologic properties and the incoming percolation flux.

For the drift-scale flow model used for calculating seepage, the fracture hydrologic properties were defined in the same way as for the mountain-scale flow model (Bodvarsson et al. 1997, Chapter 7). Additional information needed to define the variability of the fracture-permeability field by location was taken from a series of air-permeability tests conducted at the location of the drift-scale thermal test in the ESF.

As with the modeling of mountain-scale flow, the DKM is preferred for modeling seepage at the drift-scale. To simplify the drift scale calculations, effects of the rock matrix were not considered, and flow was calculated using a model for only the fracture continuum. This simplification is conservative compared to the DKM because the effect of including the matrix would be to decrease the fracture flow and reduce the amount of seepage (the large-capillary suction in matrix pores prevents matrix flow from seeping into drift openings). Another simplification is to assume steady-state conditions. The possibility of episodic flow and discrete-fracture effects at the repository and their effect on seepage needs further study, as discussed in Section 2.7.4.2.

In the seepage modeling, drift collapse, mineral precipitation, and thermal alteration of hydrologic properties are not considered. It is expected that the drifts will be stable for only a few hundred to a thousand years. Therefore, long-term repository performance will depend on the amount of seepage into a drift filled with rockfall rubble, rather than into an open drift. In addition, thermal-mechanical and thermal-chemical effects could alter the hydrologic properties around the drifts, possibly even permanently. Future work will include the study of effects of drift collapse and thermal alteration of hydrologic properties.

2.3 KEY ISSUES ASSOCIATED WITH PROCESS MODELS

2.3.1 Development and Prioritization of Issues

As part of the preparation for TSPA-VA, a 3-day UZ-flow workshop was held on December 11–13, 1996, in Albuquerque, New Mexico. Much of the time in the workshop was spent discussing the current state of knowledge of UZ flow in Yucca Mountain and the important issues relevant to UZ flow. A list of these issues was compiled by the participants (who included a broad cross-section of data gatherers, process modelers, PA subsystem modelers, and TSPA modelers from within the Yucca Mountain Project), followed by discussion of priorities and approaches to dealing with the issues in TSPA-VA (Altman et al. 1997, Chapter 5).

Before the workshop, the Abstraction Core Team (ACT) prepared a list of issues for the participants to address. These issues, in the form of questions, are listed below:

1. What (range of) infiltration should be used for TSPA calculations?

2. Should the model(s) have a significant amount of lateral diversion above and below the repository?

3. How should the perched water be modeled?

4. How should fracture/matrix interactions be modeled?

5. How should flow channels be modeled?

6. How should seepage into drifts be modeled in TSPA calculations?

7. What (range of) matrix properties should be used?

8. What (range of) fracture properties should be used?

9. With what observations do the model(s) need to be consistent?

10. What numerical formulation of conceptual model(s) should be used for TSPA calculations (e.g., ECM, GECM, DKM, Weeps)?

The issues were then addressed, consolidated, and prioritized into four categories during the workshop as shown in Table 2-4. The criteria for prioritization were as follows:

1. Does the issue have a strong effect on percolation flux at the repository?

2. Does the issue have a strong effect on seepage into the drift?

3. Will the issue be important to flow and transport below the repository?

4. Does the issue have a strong effect on the partitioning of flow between the fractures and matrix?

These criteria were chosen based on results of past PAs and the sensitivities of calculated peak doses to these criterion. Details of the prioritization and compilation of the issues can be found in Altman et al. (1997).

In addition to those issues in Table 2-4, some issues were considered to cut across the categories listed in the left column of Table 2-4. Cutting across categories 1 and 2 were the following:

- Does grid-scale heterogeneity need to be included?
- Should sub-gridblock-scale fractures be lumped with the matrix?
- How should matrix properties be upscaled?
- How should uncertainty in upscaling be propagated?
- How should spatial variability in the parameters be included?

Cutting across categories 2 and 3 in Table 2-4 was:

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

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

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

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

There was also an integration issue: "How are different models for TH, flow, and transport handled?" Resolution of this issue has required close cooperation among the UZ-flow, UZ-TH, and UZ-radionuclide-transport groups.

The issues listed above (from Table 2-4) have almost all been considered in TSPA-VA to some extent. However, two of the issues require field or laboratory experiments and are thus beyond the workscope of TSPA. These issues are "How representative are the isotopic and water-chemistry data?" and "What features, processes, and parameters affect fracture/matrix interactions (coatings, connectivity, aperture, flux, etc.)?" Addressing these issues would add to the defensibility of the TSPA calculations. In TSPA-VA, measured isotopic abundances and water chemistry are assumed to be representative of the system as discussed in Fabryka-Martin et al. (1998, pp. 93-96). The assumptions about the representativenes of the measured isotopic and water-chemistry data are detailed in that report, and the relevant basis for UZ flow models in TSPA-VA is addressed in Section 2.6.1.2.1, where 50-year fast flow paths are compared among different conceptual models of unsaturated flow at Yucca Mountain. Fracture-matrix interactions have been addressed through numerical studies that assess different conceptual models of interactions between fractures and matrix and their effects (Ho 1997, Introduction; Bodvarsson et al. 1997, Chapter 5). To ground these sensitivity studies with laboratory experiments would add strength to the models.

Another list of important UZ-flow issues has been generated (Barr et al. 1995, pp. 56-85), as part of a larger project to catalog features, events, and processes (FEPs) that are important to performance of a Yucca Mountain repository. The correspondence between the nominal-flow FEPs and the important issues listed in Table 2-4 is not transparent for two reasons. First, UZ-flow as defined for TSPA-VA is only a subset of the "nominal" FEPs, which include thermohydrologic and surface-runoff processes, for example. Second, the issues in Table 2-4 and the FEPs in Barr et al. (1995) are at different levels of detail; the list above contains many rather specific modeling issues, for example, whereas the FEP "trees" are more general. We believe that all purely UZ-flow FEPs are being captured in TSPA-VA, either explicitly or implicitly. It is also important to note that while the FEPs reported in Barr et al. (1995) are useful for providing *guidance* to important scenarios, they are not currently used exclusively as the *basis* for design- or licensing-related activities.

2.3.2 Analysis Plans and Site Investigations to Address Key Issues

A number of issues in Table 2-4 have been addressed in sensitivity studies developed through analysis plans outlined in the workshop. The analysis plans were designed to address the important issues listed in Table 2-4 with the goal of providing useable products and information for TSPA-VA. Section 2.4 details the analyses that have been performed to date and the incorporation of these studies into TSPA-VA. Several issues that arose in the workshop, but which are not addressed in Section 2.4, are listed below and addressed in the following paragraphs:

- Effects of intra-unit heterogeneities on UZ flow
- Use of different formulations of fracture characteristic curves
- Fracture-matrix interactions at unit boundaries
- Calibration using a three-dimensional model versus one-dimensional columns.

Although the effects of intra-unit heterogeneities have not been investigated in the LBNL three-dimensional site-scale model, Altman et al. (1996, pp. 117-123) provided results of heterogeneous groundwater travel-time simulations of two-dimensional cross-sections of Yucca Mountain. Their findings showed that the intra-unit heterogeneities (implemented through geostatistical methods) yielded distributions of travel times that spanned several orders of magnitude about the mean values. While this is an important finding, the current approach attempts to capture the distribution of travel times through the UZ via the use of different DKM conceptual models that approximate fast flow paths through fractures.

The identification of accurate fracture characteristic curves is difficult to obtain. Measurements of capillary pressure and relative permeability in fractures have been sparse, so sensitive fracture parameters (e.g., fracture-matrix interaction parameters) are treated as fitting parameters during the UZ flow calibrations (see Section 2.4.3.1.3). Fracture-matrix interactions at unit boundaries are also difficult to ascertain, so calibrations are used to gain confidence in the treatment of fracture-matrix interactions throughout the model domain.

Current calibrations rely on inverse models using one-dimensional columns (see Section 2.4). Optimized hydrologic parameters are then used in three-dimensional models and further refined to accommodate perched water and other observed data (see Section 2.4.3.1.3 and Section 2.4.3.4). Results of the three-dimensional simulations are checked against one-dimensional calibration data to ensure that calibrated parameters from the one-dimensional simulations are still valid in the three-dimensional model.

Field Tests

Many of the issues in Table 2-4 have also been addressed by the current field-testing program, although not all of the planned tests were completed in time to be used in TSPA-VA. Some of the field tests are briefly described below.

Niche studies were carried out to investigate seepage into drifts. These studies evaluated ambient seepage by closing off niches in the ESF and monitoring inflow of water (if any) and changes in hydrological conditions in the walls of the niches. Active water and tracer tests were also being conducted, with water and tracers being introduced above the niches. The results of the active tests provided seepage rates as a function of the total introduced percolation rate, which was used to calibrate the models for seepage into drifts.

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

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

2.4 ABSTRACTION APPROACH AND IMPLEMENTATION

The abstraction approach and implementation of UZ flow models for TSPA-VA were motivated by components and issues of UZ flow and UZ-flow modeling that have been identified as potentially important to PA calculations of Yucca Mountain (Table 2-4). Important issues detailed in the previous section were addressed in abstraction and testing analyses that fall into four areas: (1) climate, (2) infiltration, (3) mountain-scale UZ flow, and (4) drift-scale seepage. The following sections describe important issues and components in each of these areas and their implementation in TSPA-VA.

2.4.1 Climate

The TSPA-VA required future-climate scenarios to define boundary fluxes and water-table elevations for UZ- and SZ-flow modeling. The boundary fluxes were determined through infiltration models that used MAPs supplied by the climate models. The strategy for TSPA-VA was to use a reasonable LTA climate as the basis for the calculations with excursions to more extreme climates. The assumption was that if the performance was sensitive to these excursions, the importance would be noted in TSPA-VA and examined in more detail in TSPA-LA. This strategy followed from the premise that future climates within a local geographic area are presently unpredictable except possibly in a relatively imprecise manner. (An alternative strategy is to use a worst-case climate in the TSPA-VA calculations, with the assumption that if performance is adequate for this climate it must be adequate for less extreme climates. This strategy was rejected because postulated worst-case climates occur very infrequently and probably not at all in the near future before radioactive decay has substantially reduced the radionuclide inventory of the repository. Thus, a worst-case climate would not allow a realistic assessment of performance.)

2.4.1.1 Discrete Climate States

Future climate was modeled in TSPA-VA as a sequence of discrete steady states. Only three discrete climate states were considered for TSPA-VA to accommodate modeling efforts: present, LTA, and superpluvial. Present climate represented relatively dry, interglacial conditions. The LTA represented the typical conditions at Yucca Mountain, between the wet and dry extremes. Because glacial climates dominated globally over the last million years, the LTA represented an average pluvial period at Yucca Mountain. The superpluvial represented periods of extreme wetness, e.g., the Stage 6 glaciation. Superpluvials were expected to occur less frequently than the 100,000-year glacial cycle (CRWMS M&O 1998, *Yucca Mountain Site Description*, Section 4.3). Values for MAP during each of the three climates are given in Table 2-5. Justification for these parameters was based on paleoclimate reconstructions from available data from the local region: pack-rat middens, lacustrian deposits, lake levels, etc. (CRWMS M&O 1998, *Yucca Mountain Site Description*. Sections 4.1 and 4.2).

Anthropogenic climates (i.e., global warming) are speculative, although supported by some global-climate modeling and the general increase in global temperature noted this century. These climates were estimated at Yucca Mountain to produce precipitation rates approaching the LTA. This estimate was based on the possibility of near-continuous El Niño conditions developing (e.g., Trenberth and Hoar 1996) and the near doubling of precipitation that accompanies these conditions at Yucca Mountain. (The increase in precipitation associated with El Niños can be estimated by examining the recent precipitation records in Table 4.1-26 of CRWMS M&O 1998 *Yucca Mountain Site Description*, realizing that 1983, 1987, 1990, 1992, 1993, and 1995 were years affected by El Niños. For example, Amargosa Farms has approximately 70% higher precipitation in those years than in the non-El Niño years.) Therefore, any global-warming impact on future climates is considered to be similar to the LTA precipitation. In fact, infiltration might be different for global warming as compared to LTA because the temperature would be higher (expected to be about 2°C, or 4°F, warmer than currently and more than 5°C, or 9°F, warmer than the LTA [CRWMS M&O 1998, *Yucca Mountain Site Description*, Section 4.2]), but effects of these temperature differences were not considered in TSPA-VA. These effects will be addressed in future TSPAs, as appropriate.

Infiltration rates were determined for each of the climates (dry, LTA, and superpluvial) using the YMP infiltration model (Section 2.4.2). The results from the YMP infiltration model were justified by comparing them with independent recharge estimates (e.g., recharge based on the Maxey-Eakin method and recharge measured at Rainier Mesa). Water-table rise above the present level was taken to be 80 m for the LTA (based on Sr-data from the Calico Hills), and 120 m for the superpluvial (based on an estimate of water-table rise for paleosprings in the vicinity). These input values were used by LBNL with the three-dimensional LBNL UZ flow model to determine flow fields for TSPA-VA.

2.4.1.2 Uncertainty

For TSPA-VA, uncertainty in future climates was represented by including uncertainty in the infiltration rates. The YMP UZ flow model has been used to calculate flow fields, using the expected present-day infiltration map (Section 2.4.2), as well as to calculate variations about the expected map. The present-day infiltration map was multiplied and divided by three in the base case to include uncertainty in the infiltration values (see Section 2.4.2.7 and Section 2.4.2.9 for more details). The infiltration maps corresponding to the LTA and superpluvial climates were similarly divided and multiplied by three in the base case to develop lower-bound and upper-bound infiltration rates. (Note that by using a multiplier, the variance for these distributions—i.e., the separation between the lower and upper bounds—increases with increasing average infiltration.) The UZ flow model was used to generate flow fields for these cases, and sampling of these flow fields in TSPA-VA calculations was weighted the same as for the present-climate flow fields. Sensitivity studies also considered increased uncertainty in the infiltration maps by using factors of five instead of three (see Section 2.6.1.1).

Because of the time scales involved, a measure of uncertainty in mean climate precipitation is not presently available; in TSPA-VA, interannual precipitation variability is used as an estimate of climate precipitation uncertainty. Interannual variability (defined as one standard deviation from the mean) in precipitation in the State of Nevada over the last 100 years has been between 20% and 30% (DeWispelare et al. 1993, p. G1-2). Arid and semi-arid regions can have interannual variability of 50% (DeWispelare et al. 1993, p. G2-3). A value of 50% uncertainty in mean climate precipitation was assumed for TSPA-VA. Therefore, although the mean precipitation for the LTA climate is estimated to be 300 mm/yr, it could be as low as 150 mm/yr ($0.5 \times 300 = 150$) and as high as 450 mm/yr ($1.5 \times 300 = 450$). Estimated uncertainty ranges for the three climate states considered in TSPA-VA are listed in Table 2-6. Note that the Maxey-Eakin method, although a nonlinear function of infiltration and precipitation, gives approximately a factor of three increase in infiltration with a 50% increase in precipitation at the precipitation rates being considered (see Table 8-2 in Wilson et al. 1994). Thus, in TSPA-VA, the estimated range of uncertainty in mean precipitation is relatively consistent with the estimated range of uncertainty in infiltration rate.

2.4.1.3 Timing

TSPA-VA calculations investigated performance periods of 10,000 years, 100,000 years, and 1 million years. The 10,000-year calculations were started with the present climate at time 0, taken to be the time the repository is closed. At a time randomly picked (i.e., picked from a uniform distribution between 0 and 10,000 years), the climate was switched to the LTA. Results indicate that the timing and duration of the climate shifts did not significantly impact the total performance (although the EBS models were not completely coupled to climate change). The abrupt changes from one climate to another caused small jumps in the dose rate due to the instantaneous changes in the water table elevation and groundwater flow rate in the SZ.

The 1-million-year calculations started with the present climate, jumped to the LTA, then either returned to the present climate or jumped to a superpluvial, and then returned to the present climate. This cycle was about 100,000 years long and thus was repeated about 10 times. Superpluvials were sampled either every other cycle or one out of every fourth cycle. Duration of present and superpluvial climates were sampled from a uniform distribution between 0 and 20,000 years; the LTA climate occurred either for the time period between the present and superpluvial, or from the present to the next present, depending on whether a superpluvial was to occur.

Table 2-7 summarizes the data used in the climate model for TSPA-VA.

2.4.2 Infiltration

A quantitative characterization of the spatial and temporal distribution of net infiltration is needed for defining upper boundary conditions for site-scale, UZ, groundwater flow models in TSPA-VA. Net infiltration is defined as the downward rate of water percolation immediately below the zone of evapotranspiration; it is not necessarily equivalent to the rate of recharge to the underlying SZ. A site-scale net infiltration model was developed to provide temporally and spatially detailed estimates of net infiltration rates over the area of Yucca Mountain and the LBNL/United States Geological Survey (USGS) three-dimensional UZ groundwater flow model (Bodvarsson et al. 1997, pp. 3.1 through 3.9; Wittwer et al. 1992). The net infiltration model is primarily a deterministic model of surface and near-surface hydrologic processes, although climatic input is modeled as both deterministic and stochastic processes. All major components of the water balance are solved in daily time increments. Daily results are provided for specified locations for analyzing the temporal distribution of net infiltration. Estimates of present-day and potential future net-infiltration rates are provided as detailed mappings of temporally and spatially varying time-averaged fluxes, which can then be applied to define upper-boundary conditions for the UZ.

The net-infiltration model simulates the water content of the soil profile by solving the water balance using daily precipitation input, modeled potential evapotranspiration, and modeled actual evapotranspiration as a function of potential evapotranspiration and available water in the soil profile. The form of the water balance used is based on the principle of conservation of mass for water at the ground surface:

$$P+\Delta W_s+R_{on}-R_{off}-D-E-T=0 \qquad (2\text{-}1)$$

where P is precipitation, ΔW_s is change in soil water storage, R_{on} is surface run-on, R_{off} is surface runoff, D is deep drainage or net infiltration, E is evaporation, T is transpiration. To be applied, Equation (2-1) must be defined over some arbitrary time interval (i.e., day, year) and over some arbitrary volume or depth in the soil.

The model in Equation (2-1) incorporates detailed geospatial data for each node to calculate the daily water balance of the soil profile using daily precipitation input and modeled potential evapotranspiration. Net infiltration is initiated by the model when the water content of the soil profile exceeds a volume determined by the soil depth and the soil-field capacity. Once net infiltration is initiated, it is limited by the effective saturated permeability of the underlying bedrock. Water available for net infiltration is also removed by modeled evapotranspiration. A modified Priestley-Taylor equation is used to model evapotranspiration as a function of the water content of the soil profile and potential evapotranspiration, which is determined from the energy balance (Flint and Childs 1991, pp. 247-260). The energy balance is primarily a function of modeled solar radiation (Flint and Childs 1987, pp. 233-248), which is solved on an hourly basis using the position of the sun, ground-surface slope and aspect, shading from surrounding topography, and atmospheric parameters for a given geographic position and elevation. Evapotranspiration is allowed to continually remove water from the soil profile to a maximum soil depth of 6 m until the residual water content for the given soil type is reached. Precipitation exceeding the storage volume of the soil profile, as determined by soil depth and porosity, is modeled as runoff and distributed to channel nodes. In the initial version of the infiltration model, the distribution of runoff to channel nodes is modeled empirically and, although the overall mass balance is satisfied, is not directly integrated with the daily water-balance calculation. Net infiltration along channel segments increases as the magnitude of simulated runoff increases, but the lateral re-distribution of surface water along sideslopes is not accounted for, and runoff is distributed uniformly across channel segments. The initial version of the infiltration model consists of a regular grid of independent one-dimensional infiltration models or nodes. A modified version of the infiltration model, scheduled to be completed in 1998, will provide an interactive grid by using dynamically coupled infiltration and surface flow routing, thus allowing for a three-dimensional representation of the natural system.

2.4.2.1 Modeling Domain, Boundaries, and Geospatial Parameters

The model domain is defined by a regular grid of 253,597 nodes consisting of 691 rows and 367 columns evenly spaced at 30-m increments aligned with the x-y axis. This grid corresponds to the 1:24,000-scale (7.5-minute quadrangle) USGS digital elevation data available for Yucca Mountain. The area of the model domain defined by this grid is a 228 km^2 rectangular region bounded by the UTM (Zone 11) coordinates of 544661 to 555641 m easting and 4067133 to 4087833 m northing (Figure 2-7 and Figure 2-8). Ground-surface elevation, slope, aspect, blocking ridges (the angle of inclination to the horizon at every 10-degree arc in the horizontal plane), bedrock geology, soil type, soil depth, and geomorphology (ridgetop, sideslope, terrace, or channel location) are defined for each node. Slope, aspect, and blocking ridges are calculated using the digital elevation model. Elevation is also used to define the spatial distribution of daily precipitation using modeled correlations between precipitation and elevation (Hevesi et al. 1 992). Bedrock geology is defined using available geospatial coverages of digitized geologic maps. For the initial version of the model, the digitized geologic map of Scott and Bonk (1984) is used for the central portion of the modeling domain covering the potential repository site and most of the area of the three-dimensional, site-scale groundwater flow model. For the remaining nodes outside the area of the Scott and Bonk coverage, the digitized geologic map of Christiansen and Lipman (1965) is used to define bedrock geology. In the initial version of the model, soil depth is assigned to each node using four soil depth classes based on a combination of quaternary surficial deposits maps Lundstrom et al. (1993a, b, 1994, 1995) and ground-surface slope. Constant soil depths are assigned to each depth class, resulting in four discrete soil depths of 0.5 m, 1.5 m, 4.5 m, and 6 m (the maximum depth of net infiltration in the initial version of the model). A more detailed mapping of soil depth is scheduled to be completed in 1998. Soil type is assigned to each node using a recombination of soil types mapped by Lundstrom et al. (1993a, b, 1994, 1995) into 10 soil types having different hydrologic properties.

The model uses a second input file for assigning effective permeability and porosity to each geologic unit and for assigning porosity, residual water content, field capacity, and saturated permeability to each soil type. The effective permeability for bedrock is a weighted average of saturated-matrix permeability, as determined from laboratory analysis of core samples (Flint 1998, pp. 44-45), and estimated fracture permeability determined using an estimated average fracture size (Wilson et al. 1994, Chapter 7, p. 29) and laboratory analysis of the saturated permeability of fracture fillings. The weighting of the matrix and fracture permeabilities is defined using an estimated fracture density. Soil porosity and saturated permeability were measured for each soil type using a combination of field testing and laboratory analysis of soil samples (Hofmann et al. 1993). Residual water contents and field capacities for each soil type were determined using a combination of fitted and derived van Genuchten water-retention curves (the derived curves were obtained using empirical models based on soil texture, which was measured). The mathematical expressions for the van Genuchten curves are presented in Section 2.4.3.2.4, and the curves are illustrated in Figure 2-6.

2.4.2.2 Model Calibration

The initial version of the infiltration model was calibrated using the 1984–1995 record of measured water-content profiles from approximately 80 neutron access boreholes and a developed record of daily precipitation for 1980–1995 (Flint et al. 1996). Records from boreholes identified as potentially problematic because of the accelerated downward percolation of water along the annular space were excluded. Model calibration consisted of both qualitative and quantitative comparisons of measured versus simulated water-content changes for the soil profile. The model-calibration process involved primarily adjustment of the parameters defining the modified Priestley-Taylor equation so that a satisfactory fit between measured and simulated time-dependent changes in soil moisture over 2- to 11-year periods was obtained on average for all borehole locations considered (length of record varies between boreholes). Additional calibration of the modified version of the infiltration model will consist of comparing time series of measured and simulated streamflow volumes, and also comparing time series of improved field estimates of evapotranspiration with simulated estimates. Annual statistics for precipitation (using the developed daily precipitation record), net infiltration, and runoff obtained using the calibrated model for the 1980–1995 simulation are listed in Table 2-8.

2.4.2.3 Stochastic Simulation of 100-Year Daily Precipitation Input using Analog Current and Potential Future Climates

The primary input driving the infiltration model is daily precipitation. Daily precipitation input is obtained using available records or is generated using a stochastic model of daily precipitation. Most of the long-term precipitation records in the Yucca Mountain region (southern Nevada and southeastern California) consist of less than 50 years of complete record. Precipitation models, which are used to generate longer precipitation records, are applicable to a Monte Carlo analysis of net infiltration and also allow for the simulation of paleoclimates, which may not have present-day analogs. A stochastic model of daily precipitation developed for the net infiltration model uses a third-order Markov chain to determine the probability of the occurrence of daily precipitation. The 32 transition probabilities for a third-order, two-state Markov chain model of the occurrence of measurable daily precipitation are estimated for each month by the equation (Gregory et al. 1992, pp. 1443-1446; Gregory et al. 1993, pp. 299-310; Haan 1977, pp. 302-309):

$$P_{ij}^{q} = \frac{n_{ij}^{q}}{\sum_{j=1}^{m} n_{ij}^{q}} \tag{2-2}$$

where P is the transition probability, q is the month, and n is the number of times state i transitions to state j. The model uses a 4-day sliding window to determine the probability of precipitation occurrence following a sequence of wet or dry days for the three preceding days. In general, the results define the probability of precipitation on the fourth day given a known state of precipitation for the preceding 3 days. Once the occurrence of precipitation is simulated, the magnitude of daily precipitation is determined using a modified exponential type cumulative-probability distribution function:

$$P_S = e^{(-A_S (PPT)^{B_S} + A_S)} \tag{2-3}$$

where P is the cumulative probability for a month or season, S, of daily precipitation amount, PPT (hundredths of inches), and A and B are fitted parameters. The parameters are determined using nonlinear least squares fitting of the modified exponential model to the sampled monthly (or seasonal) cumulative-probability distribution function of daily precipitation magnitudes.

To define parameters for a stochastic daily precipitation model representative of the current climate at Yucca Mountain, a 36-year record of daily precipitation from the Nevada Test Site station 4JA located approximately 15 km east of the potential repository site was used. Although this site is lower in elevation than the potential repository site, this station provides the longest near-continuous record of daily precipitation in the close proximity of the potential repository site. Simulated daily precipitation amounts for 4JA were scaled to the Yucca Mountain site using a combination of topographic scaling and the ratio of average annual precipitation for the two locations. Table 2-9 provides a comparison of average annual precipitation calculated using measured daily precipitation at 10 stations located within the modeling domain with average annual precipitation obtained using topographic scaling and the scaled 4JA model of daily precipitation, and also with average annual precipitation obtained using topographic scaling and the 1980–1995 developed record of daily precipitation. Values obtained using the model are for the 30-m grid nodes closest to the location of the precipitation stations. Estimated values of average annual precipitation indicate a reasonable overall match to values obtained using the precipitation records at 7 stations with 8 or more years of record, as indicated by a comparison of the global mean obtained for these locations (157 mm calculated versus 149 estimated using the scaled 4JA record and 156 mm estimated using the 1980–1995 developed precipitation record). The variability between estimated values and values calculated from the available records at specific locations is likely due to local-scale terrain effects on precipitation, such as site exposure (including slope, aspect, and surrounding topography), which are not accounted for by a model based only on site elevations. Additionally, some variability between estimated values and values obtained using available records is expected because of differences in both the length and period of record. For example, the period 1989 through 1996 provides a better match to estimates obtained using the 1980–1995 developed precipitation record because these periods are characterized by a similar frequency of wetter than normal years which were likely caused by an increased frequency of the El Niño Southern Oscillation. In comparison, the 100-year scaled 4JA simulation tends to be drier because the 1957 through 1993 4JA record is drier overall than the 1980–1995 period. The sensitivity of calculated values of average annual precipitation to both the length and period of record is indicated by a comparison of the three sites with only four years of record. The 1993–1996 period is characterized by two wetter than normal years (1993 and 1995), which have probably biased the calculated values (they are expected to be higher than longer term averages). In general, 4 years is not considered an adequate length of record to calculate average annual precipitation, especially in arid climates where year to year variability in precipitation is high (French 1987).

To define the parameters for the analog potential future climates, daily-precipitation records from three different locations (Area 12 Mesa, South Lake, and Lake Valley–Steward) in the south-central Basin and Range were used. Area 12 Mesa is located on Rainier Mesa in the northern part of the Nevada Test Site; Lake Valley–Steward is located close to Pioche in eastern Nevada; and South Lake is located on the eastern slope of the Sierra Nevada in California (Figure 2-9). All locations are at higher latitudes and elevations relative to Yucca Mountain, and they were assumed to be representative of approximate analogs to potential future climates based on mean annual precipitation values shown in Table 2-5. Although these analog sites have yet to be rigorously evaluated in relation to the expected characteristics of predicted future climates (for example, the expected seasonal distribution of precipitation), the Area 12 Mesa and the Lake Valley–Steward sites are assumed to be approximate analogs to a potential LTA future climate having a mean annual precipitation rate of 300 mm/yr. The South Lake site is assumed to be an approximate analog to a potential superpluvial future climate having a mean annual precipitation rate of 450 mm/yr (CRWMS M&O 1998, *Yucca Mountain Site Description*. Sections 4.1 and 4.2). (If further evaluation shows that estimations of precipitation (and temperature) at these analog sites are not representative of predicted future climates, then alternative sites and/or models should be considered to maintain a defensible system.) To provide a simulation for a potential upper bound (wettest) future climate, simulated daily precipitation values defined by the South Lake site were scaled by a factor of 1.581, which resulted in the desired modeled analog climate with an average annual precipitation rate of 675 mm/yr (see Section 2.4.1.2 and Table 2-6). The South Lake site was the wettest location available from the regional network of precipitation stations in the Yucca Mountain region, and the scaling factor allowed a match between the simulated daily precipitation values and the desired upper MAP estimate in Table 2-6. Information on station records, locations, elevations, statistical summaries obtained from the daily precipitation records, and the corresponding statistics obtained for a 100-year simulation of daily precipitation for all four analog climates are listed in Table 2-10. Statistics obtained for 10 different 100-year simulations for all four analog climates are listed in Table 2-11.

2.4.2.4 Modeled Net-Infiltration Results Using a 100-Year Simulation of an Analog Current Climate for Yucca Mountain

Figure 2-10 indicates the spatial distribution of average net infiltration rates for the modeling domain using a 100-year stochastic simulation of current climate for Yucca Mountain (the scaled 4JA model). The average simulated net infiltration rate for the entire area of the modeling domain is 3.25 mm/yr, and a maximum rate of 63 mm/yr is obtained for a relatively high-elevation location on the prow of Yucca Mountain. Simulation results showed net infiltration values of 0 mm/yr for all nonchannel locations having a soil depth of 6 m or greater. The average net infiltration rate for channel nodes is 9.2 mm/yr. To analyze simulation results for areas overlying the potential repository site, statistics for three different subareas are compared (Figure 2-11). Table 2-12 lists summary statistics of net infiltration simulations for the entire modeling domain and the three subareas obtained using results for the 100-year current climate simulation and the original scaled 1-year simulation of current climate for Yucca Mountain. Results obtained for the 100-year simulation of current climate are similar to the original scaled 1-year simulation of current climate, although results obtained for the 1-year simulation are on average slightly higher than the 100-year simulation.

To analyze the temporal variability of modeled net infiltration, daily results obtained using the 100-year current climate simulation were extracted for the 30-m grid node centered over the location of borehole SD-9 (refer to Figure 2-49 later in this chapter, for location of boreholes). For comparison, results were also obtained for the 3 × 3 cluster of grid nodes centered on the SD-9 location. Results were obtained for three separate 100-year stochastic simulations for both the single node and the nine-node cluster in order to analyze the sensitivity of the results to differences in daily precipitation input for the 4JA analog climate, as well as the sensitivity of results to differences in geospatial parameters for adjacent nodes. As indicated in Table 2-13, simulated average net infiltration rates vary from 7.56 to 10.86 mm/yr for the single-node case, and from 2.42 to 3.65 mm/yr for the nine-node cluster, depending on which 100-year stochastic simulation is used. The variability in results between the single node and nine-node cluster reflects the high degree of spatial variability in estimated net infiltration which can exist at a given location within the modeling domain. Variability in estimated values between adjacent grid nodes is dominantly caused by differences in soil depth, bedrock geology (effective permeability of bedrock varies by several orders of magnitude), soil type, and topography (slope, aspect, elevation). This variability can be an important consideration in hydrologic analysis at specific locations, such as comparisons of borehole data with net infiltration estimates, and especially in situations where vertical ground water flow should not be assumed. However, such local-scale variability may not be important on the scale of the UZ ground water flow modeling domain. Because the UZ model mesh is coarser than the 30-m node spacing of the net infiltration model, local-scale variability is smoothed when net infiltration estimates are interpolated onto the coarser mesh. Such smoothing may actually be representative of local-scale lateral flow processes in the shallow subsurface (the net infiltration model extends to a depth of only 6 m) which would tend to cause a dampening of locally variable net infiltration rates. However, it should be noted that such a conceptualization may not be applicable if localized fast pathways exist.

Simulated average annual precipitation at SD-9, calculated from the 100-year simulations of daily precipitation, varied from 157 mm for the single-node case to 158 mm for the nine node cluster (although simulated daily values were different for each of the three stochastic simulations, the double scaling method used to transpose the 4JA results to Yucca Mountain scales daily values based on estimates of average annual precipitation, which causes calculated average annual precipitation for each stochastic simulation to be equivalent). Only one of the simulations resulted in the generation of runoff for this location (0.16 mm/yr for the single node and 0.05 mm/yr for the nine-node cluster). Maximum annual net infiltration varied from 140 mm to 73 mm for the single-node case, while maximum daily net infiltration varied from 35 to 65 mm. Maximum daily evapotranspiration varies from 1.76 mm for the single-node case to 1.39 mm for the nine-node cluster.

The annual variability of simulated precipitation, evapotranspiration, change in soil water content, and net infiltration at the SD-9 location, using stochastic simulation #2 for the single-node case is indicated in Figure 2-12. On average, net infiltration occurs for only approximately 1 out of 7 to 10 years, although a well defined cycle is not apparent for the simulation (because the stochastic simulation is modeled as a purely random process, annual cycles appear only by coincidence). Although the maximum annual net infiltration of 140 mm occurred for the year with the maximum annual precipitation of 371 mm, annual net infiltration is not linearly dependent on the magnitude of annual precipitation. For example, year number 35 has a relatively high annual precipitation of 267 mm, but is a year with no net infiltration because most of the precipitation occurs during the summer and because the preceding 2 years are relatively dry, with annual precipitations of 64 and 67 mm, respectively.

2.4.2.5 Modeled Net Infiltration Results Using 100-Year Simulations of Analog Potential Future Climates for Yucca Mountain

Estimates of average net infiltration rates obtained using the Area 12 Mesa, the Lake Valley–Steward, the South Lake, and the scaled South Lake analog wetter climate 100-year simulations are indicated in Figure 2-13, Figure 2-14, Figure 2-15, and Figure 2-16, respectively. A summary of simulation results for all four analog potential future climates, according to the full modeling domain and the three subareas overlying the potential repository site, is given in Table 2-14. Results for the Area 12 Mesa simulation include a spatially averaged mean of 19.72 mm/yr for the modeling domain and a maximum rate of 275.34 mm/yr for a location in the headwaters of Drillhole Wash. The simulated mean estimate of 19.72 mm/yr is in good agreement with estimates of recharge obtained for study sites located close to the Area 12 Mesa precipitation station on Rainier Mesa in the northern part of the Nevada Test Site. Average annual net infiltration for the area of the potential repository (Subarea 5) is estimated to be 32.66 mm/yr, with a maximum estimate of more than 150 mm/yr for several locations in the headwaters of washes. The spatially averaged net infiltration rate for the areas of Split and WT-2 Washes (Subarea 3) is 28.80 mm/yr, and the maximum rate is 169.22 mm/yr obtained for a channel location. Average net infiltration along stream channels is estimated to be 76.96 mm/yr, assuming that 50% of the runoff generated contributes to net infiltration along channels. This assumption is based on preliminary results of a coupled infiltration/surface-flow routing model that has been developed by the USGS. Average annual runoff depth for the study area, using the Area 12 analog site, is 8.69 mm/yr, with a maximum value of 144.389 for a location along the northern boundary of the grid. Minimum net infiltration estimates of 0 mm/yr are obtained for most, but not all, locations with deep soils. Values of net infiltration are greater than 0 for the alluvial fan in the upper part of Yucca Wash, whereas estimates of 0 mm/yr are obtained for these locations using the scaled 4JA analog current-climate simulation.

Estimates of average net infiltration rates obtained for the 100-year simulation using the Lake Valley–Steward analog potential future climate include a spatially averaged mean of 31.22 mm/yr for the modeling domain and a maximum rate of 390.75 mm/yr for a location in the headwaters of Drillhole Wash (Figure 2-14). The average net infiltration rate for channel nodes is 120.63 mm/yr (assuming 50% of runoff generated contributes to net infiltration along channels). For the area of the potential repository (Subarea 5), the average net infiltration rate is 49.8 mm/yr, the maximum rate is 244.4 mm/yr (obtained for a channel location), and the minimum rate is 1.4 mm/yr. The spatially averaged net infiltration rate for the areas of Split and

WT-2 Washes (Subarea 3) is 44.1 mm/yr and the maximum rate is 169.22 mm/yr obtained for a channel location.

Estimates of average annual net infiltration obtained using the 100-year stochastic simulation for the South Lake analog wetter climate site, which provides a spatially distributed average annual precipitation rate of 427.06 mm/yr, includes a spatially averaged mean of 81.02 mm/yr for the modeling domain and a maximum rate of 847.69 mm/yr for a channel location in upper Yucca Wash (Figure 2-15). The estimated average annual runoff depth resulting from the South Lake analog wetter climate is 52.30 mm/yr. Assuming that 50% of the total runoff volume contributes to net infiltration along channels, an average net infiltration rate of 663.06 mm/yr is calculated and added to net infiltration from precipitation at channel locations, providing the maximum rate of 847.69 mm/yr. The spatially averaged net infiltration rate obtained for the area of the potential repository (Subarea 5) is 108.00 mm/yr, with a maximum rate of 706.49 mm/yr occurring at channel locations. The spatially averaged net infiltration rate for the area of Split and WT-2 Washes (Subarea 3) is 105.56 mm/yr.

In contrast to results obtained using the scaled 4JA, the Area 12 Mesa, and the Lake Valley–Steward analog climates, results obtained using the South Lake analog climate indicate positive (greater than zero) average net infiltration rates for the entire area of the grid, including the deep soils of the alluvial fans. The relative control of the effective permeability of the bedrock on net infiltration is stronger than the control of soil depth or even the spatial distribution of precipitation; for the scaled 4JA current climate and the Area 12 potential future climate simulations, the relative control of bedrock permeability was secondary to soil depth and the spatial distribution of precipitation. The South Lake simulation indicates that the significance of maximum net infiltration rates occurring throughout the channel network is much greater than for drier climates, with net infiltration along channels accounting for a relatively greater proportion of total areal net infiltration volumes. These simulations do not take into account changes in vegetation, soil cover, and climatic parameters such as air temperature and cloud cover that would be expected in conjunction with the wetter conditions. In addition, depending on the increase in the height of the regional water table and/or local perched-water tables, some parts of the study area would likely become zones of discharge, as opposed to zones of net infiltration or recharge under such wet conditions.

Estimates of average annual net infiltration obtained using the 100-year stochastic simulation for the scaled South Lake analog wetter climate site, which provides a spatially distributed average annual precipitation rate of 675 mm/yr, includes a spatially averaged mean of 250 mm/yr for the modeling domain and a maximum rate of 2,080 mm/yr (Figure 2-16). The simulated average annual runoff depth obtained using the scaled South Lake climate is 154 mm/yr. Assuming that 50% of the total runoff volume contributes to net infiltration along channels, an average net infiltration rate of 1,360 mm/yr is calculated and added to net infiltration from precipitation at channel locations. The averaged net infiltration rate obtained for the area of the potential repository (Subarea 5) is 229 mm/yr, with a maximum rate of 1,830 mm/yr occurring at a channel location. The spatially averaged net infiltration rate for the area of Split and WT-2 Washes (Subarea 3) is 242 mm/yr. In general, the scaled South Lake 100-year simulation indicates a transition in the spatial distribution of net infiltration, with maximum rates shifting from upland areas to the alluvial fans (excluding the maximum rates that occur at channel locations). The spatial pattern of net infiltration rates primarily reflects the effective conductivity of the underlying bedrock. For deep alluvium (> 6 m thickness), the underlying bedrock is modeled as alluvium, which has a relatively high effective conductivity. The model does not take into account lateral flow below a depth of 6 m which would likely occur along the alluvium-bedrock contact under such wet conditions, depending on the permeability of the bedrock underlying deep alluvium. Limitations in the model, which were discussed for the South lake simulation results, are amplified for the wetter conditions of the scaled South Lake simulation. In general, the results obtained for the scaled South Lake simulation represent a severe extrapolation of model parameters, which were calibrated for a much drier current-climate simulation, and thus should be interpreted with great caution.

In addition to average annual net infiltration rates, simulation results were also obtained as 5-year averages, providing a sequence of twenty 5-year-average net-infiltration rates for the full modeling domain for each of the five 100-year simulations discussed above. These results provide a means of investigating the combined temporal and spatial variability in simulated net infiltration rates for the modeling domain, and allow the potential of developing dynamic, transient upper boundary conditions for a given climate. A statistical summary of the twenty 5 year average results for each climate is provided in Table 2-15. Five-year-average net infiltration rates vary from 10.95 to 0.17 mm/yr using the 4JA current-climate simulation, and from 361 to 196 for the scaled South Lake upper bound climate simulation. The relative variability (coefficient of variation) for the 5-year-average net infiltration rates decreases as the climate becomes wetter.

2.4.2.6 Discussion of Modeled Net Infiltration Results

The spatially averaged net infiltration rates obtained for the various 100-year stochastic simulations are plotted against the corresponding values of average annual precipitation for a comparison with estimates of net infiltration and recharge obtained using alternative approaches (Figure 2-17). The comparison includes the modified Maxey-Eakin model (Flint et al. 1996), the original Maxey-Eakin (1949) step function, the estimates obtained by Lichty and McKinley (1995, pp. 4-14) using both the PRMS water-balance model and the chloride-balance model, the average annual net infiltration estimate for Yucca Mountain (Flint et al. 1996) using a statistical model based on the 1984–1995 neutron logging record, and the estimate of average annual recharge for the upper Amargosa River basin obtained by Osterkamp, Lane, and Savard (1994, pp. 493-507) using streamflow simulation models. Estimates obtained using the net infiltration model are generally consistent with previous estimates of recharge in the Yucca Mountain region, although the model results tend to be higher, on average, than previous Maxey-Eakin type estimates and the basin-wide estimate obtained by Osterkamp, Lane, and Savard (1994, pp. 493-507). Results obtained using the Area 12 Mesa and the Lake Valley–Steward 100-year simulations are fairly consistent with the chloride-balance estimate of 33 mm/yr recharge obtained by Lichty and McKinley (1995) for the Three Springs basin in the Kawich Range. The scaled South Lake 100-year simulation is drier than the recharge estimate of 300 to 320 mm/yr obtained for the East Stewart Creek site studied by Lichty and McKinkley, but wetter then estimates obtained using the original Maxey-Eakin model. Model results obtained for average annual precipitation representative of the current climate at Yucca Mountain, including the 100-year mean of 3.25 mm/yr, tend to be higher than previous estimates obtained by the Maxey-Eakin method, the modified Maxey-Eakin method, and estimates obtained by Osterkamp et al.

(1994, pp. 493-507), but are lower than the estimate of 11.9 mm/yr (Flint et al. 1996) and the modeled estimate of 7.64 mm/yr obtained using the 1980–1995 daily precipitation record.

Discrepancies in modeling results can be attributed to a combination of model uncertainty, differences in the hydrologic characteristics of the various study sites, and differences in climatic characteristics, such as the timing and frequency of precipitation, which are not accounted for using a comparison based on average annual precipitation. The stochastic model of daily precipitation does not account for annual cycles or trends, such as the El Niño Southern Oscillation and greenhouse warming, which are considered to be important aspects of the 1980–1995 record. Sources of uncertainty in the numerical model include the uncertainty in the geospatial input parameters, uncertainty in the data and developed data used to calibrate the model, and limitations concerning the model's representation of physical processes. The sensitivity of modeled net infiltration to variations in soil depth, soil hydrologic properties, and the effective conductivity of the underlying bedrock, has not yet been fully assessed. The assumption of a uniform soil depth of 0.5 m for all upland areas mapped as having thin to no soil cover may not be an adequate representation of the site. Values for effective bedrock conductivity are strongly dependent on estimates based on a limited amount of data concerning fracture properties, particularly the spatial distribution of fracture properties in the near surface. Evapotranspiration of water stored in the bedrock fractures and matrix is not included in the 1996 version of the model. An estimated 2-hour storm duration used for defining summer precipitation intensities using daily precipitation input may not adequately represent short-duration, high-intensity precipitation events common in the summer, which are likely to produce significant runoff without causing a large increase in the water content of the soil profile. The modeling of the spatial distribution of daily precipitation based on topographic scaling may provide a reasonable representation of winter precipitation, but is likely not to provide a reasonable representation of summer precipitation. The effect of vegetation on evapotranspiration in response to wetter climates has not been included in the present model. The effect of other variables such as air temperature and cloud cover on precipitation, runoff, and evapotranspiration, which is likely to become more important for the analog wetter climate simulations, is also neglected in the current model. The representation of stream channels using 30-m grid nodes does not correctly define stream channel geometries, and this is likely to strongly affect simulated quantities of stream discharge and net infiltration along channel locations. The use of a rectangular modeling domain does not account for surface-water inflows from upstream drainages, which is especially problematic for estimating net infiltration along Fortymile Wash.

In general, the uncertainty of net infiltration estimates increases as the climate being used to drive the model becomes wetter, because processes that were considered negligible for current-climate simulations become much more important in wetter climates. These processes include surface-flow routing, sub-surface flow along the soil-bedrock interface, presence of groundwater discharge zones, and development of a persistent snow cover. In addition, the effects of a denser vegetation cover (especially for warmer, wetter climates) on the interception of precipitation, evapotranspiration, and soil development (affecting both soil depth and soil properties) must be accounted for as the climate becomes wetter. All simulations obtained using the 1996 net infiltration model are dependent on geospatial parameters defined for current-climate conditions, and thus all 100-year simulations using analog wetter climates involve the extrapolation of the model to some degree (the wetter the climate the greater the degree of extrapolation). Finally, changes in air temperature and cloud cover have not been included in the analog wetter climate simulations; only the daily precipitation input is changed. For these reasons, the scaled South Lake 100-year simulation, with an average annual precipitation rate of 675 mm/yr, may not be a reasonable representation of the natural system.

The modified version of the 1996 net infiltration model, scheduled for completion in 1998, will provide an improved representation of the physical processes governing net infiltration, particularly evapotranspiration and runoff routing. A fully coupled infiltration–runoff routing algorithm will allow for an interactive, three-dimensional modeling of near-surface hydrologic processes. The modeling of overland flow will provide a more accurate representation of net infiltration along channels, and will allow for model calibration using available streamflow records in addition to the neutron logging record. The modeling domain for the modified model will be defined using drainage boundaries of surface flows rather than rectangular grids. An analysis of the sensitivity of modeling results against parameters such as soil depth and the effective conductivity of the underlying bedrock will be conducted using the modified model. Given the uncertainties and limitations of the current (1996) model, estimates of net infiltration for Yucca Mountain are considered preliminary, but not unreasonable, for the area of the potential repository site (estimates along the Fortymile Wash drainage remain problematic as a result of neglected upstream inflows), and for climates with average annual precipitation rates of approximately 500 mm/yr and less (results for the scaled South Lake climate should be interpreted with caution). In general, LTA net infiltration rates obtained using all five analog climate 100-year simulations are in approximate agreement with recharge estimates obtained using a variety of approaches throughout the Yucca Mountain region. Results obtained using the scaled 4JA analog current climate 100-year simulation are in good agreement with the fully QA'd 1-year simulation of net infiltration for current climate; are in approximate agreement with the chloride balance and temperature profile modeling approaches; are calibrated to the 1980–1995 record of daily precipitation and the 1984–1995 record of water-content profiles; and are consistent with the data and estimates used to define the conceptual model of infiltration.

2.4.2.7 Infiltration Maps Used in TSPA-VA

Based on the estimated precipitation for the LTA and superpluvial climates described in Section 2.4.1.1, precipitation data from Area 12 Mesa (MAP=289 mm/yr) and South Lake (MAP=427 mm/yr) were chosen to produce future-climate infiltration maps for the UZ flow model. The present-day infiltration map was taken from data derived in Flint et al. (1996; DTN: GS960908312211.003). The models for these future-climate analogues yielded infiltration data on 30-m × 30-m grid blocks. These infiltration data were then mapped onto the surface of the LBNL UZ flow model by taking the mean of all infiltrations within a circular area equivalent to the surface area and location of a surface grid block in the UZ flow model. The infiltration maps used in the LBNL UZ flow model for the present-day, LTA, and superpluvial climates are shown in Figure 2-18, Figure 2-19, and Figure 2-20, respectively. For the nominal present-day infiltration map (I), the average net infiltrations are as follows:

- Over entire Flint/Hevesi model domain—3.8 mm/yr
- Over entire LBNL UZ-flow model domain—4.9 mm/yr
- Over only the repository area—7.7 mm/yr.

The average net infiltrations over the repository area for the LTA and superpluvial climates are 42 mm/yr and 110 mm/yr, respectively. Because there is uncertainty in the infiltration values, multipliers were used to increase or decrease the infiltration maps (for present-day, LTA, and superpluvial) by a prescribed amount in multiple realizations of UZ-flow simulations. Several iterations of simulations and discussions were conducted to identify these multipliers, and results yielded factors that ranged between three and five. For the initial round of calculations, a factor of five was used as a multiplier for the nominal infiltration map. The factor of five was somewhat arbitrary, but it was chosen to capture some of the extreme values suggested by the Expert Elicitation panel (CRWMS M&O 1997, p. 27, Section 3). Later, based on comparisons with borehole temperature data, a factor of three was chosen for the base case in TSPA-VA. The factor-of-three increase or decrease was determined by comparing the calculated mountain-scale flow fields with observed borehole temperatures (see Section 2.4.2.9). The flow model is expected to reproduce the observed temperature gradient, which is a function of infiltration. Infiltrating water introduces an advective component to the ambient heat balance, changing the temperature profile from what it would be if heat transfer were by thermal conduction only (see Bodvarsson et al. 1997, Chapter 11). If increases are greater or smaller than a factor of three, the flow model cannot reproduce the observed temperature gradient for the UZ.

To incorporate the three infiltration maps (I, I*3, and I/3) into a Monte Carlo framework for the TSPA-VA, they are assigned probabilities of occurrence. The probabilities are assigned so that the base infiltration (I) is equal to the statistical mean because the base infiltration comes from the infiltration model, which uses the project's best estimates for all the input parameters. The probability for the high-infiltration case, I*3 (base-infiltration-times-three), was determined by balancing the recommendations made by the participants in the UA Flow Expert Elicitation (UZFEE) (CRWMS M&O 1997, Table 3-1) with information such as the temperature-gradient implications discussed above (see Bodvarsson et al. 1997, Chapter 11). A 10% probability of occurrence is assigned to the I*3 case. The requirement that the "base infiltration" case be the mean of the infiltration distribution then uniquely determines the other two probabilities to be 60% for the "base-infiltration" (I) case and 30% for the "base-infiltration ÷ 3" (I/3) case. The same probabilities are used for the other climate states (LTA and superpluvial), and the climates are correlated. For example, when climate changes from dry to LTA, if dry-climate infiltration is base infiltration ÷ 3, then LTA and superpluvial infiltration are also base infiltration ÷ 3. Table 2-16 summarizes the average net infiltrations over the repository area for the different infiltration scenarios along with the associated probabilities. In the future, a more quantitative basis for the infiltration distributions is desired. The quantitative basis would be achieved by running the infiltration model in a stochastic mode to derive explicitly the uncertainty about infiltration from the input-parameter uncertainties. Additional work is also needed to properly account for the effects of temperature and vegetation changes on infiltration for future climates.

In summary, the infiltration maps used in the LBNL UZ flow model were obtained from infiltration models using precipitation data at various sites that matched estimates of MAP for present-day, LTA, and superpluvial climates. The weightings for the variations to the nominal infiltration (I, I*3, and I/3) were determined using an infiltration distribution generated by the expert-elicitation panel, combined with input from principal investigators on the project.

2.4.2.8 Transient Infiltration Study at Borehole SD-9

The objective of this study was to perform a 100-year transient infiltration simulation to investigate the sensitivity of one-dimensional UZ flow to changes in the infiltration rate. One of the goals was to determine the influence of transient infiltration at the ground surface on the liquid flow rate at the repository horizon. Simulations and source data associated with this study have been submitted to the Technical Data Base (SNT05091597001.006).

Numerical Simulator

Numerical simulations were run using the Sandia National Laboratories/New Mexico (SNL/NM) Version 3.1.1 of TOUGH2-EOS9 (this version was configured under the SNL QA program). The Equation of State 9 (EOS9) module of TOUGH2 simulates liquid flow in unsaturated porous and fractured media using a formulation of Richards' equation where gas transport can be neglected and isothermal conditions exist. A DKM in which flow is explicitly modeled in the fracture and matrix elements was used.

Model Domain and Boundary Conditions

Simulations were run on a one-dimensional column representative of the geologic conditions at the location of borehole SD-9. The one-dimensional grid used in these TOUGH2 simulations was extracted from the LBNL three-dimensional model as shown in Figure 2-21. The cross-sectional area of each grid block is 6,810 m^2. The domain consists of 22 elements. Each element represents one hydrostratigraphic unit, with the exception of TSw5, which is split into three elements, and TSw6, which is split into two elements. These layers were split into more than one element in order to further refine the grid at the approximate elevations of the repository. One modification has been made to the layering used by LBNL. In the three-dimensional model, the upper layer of the Calico Hills was modeled by LBNL as a zeolitic layer. LBNL's reasoning behind this classification was that the layer is partially altered and that only the upper 4 m of the layer can be considered unaltered. In this sensitivity analysis, the layer was changed to a vitric layer (CH1v in Figure 2-21) because the low observed saturations at that elevation suggested that there was a vitric layer there. The best solution would be to split this grid block into two so that there was a 4-m vitric layer on top. But for the purposes of this analysis, that refinement was unnecessary. The inclusion of the vitric layer allowed for water to be transferred back into the matrix in the CH1v.

Initial One-Dimensional Steady-State Equilibrium Simulation

Before the transient infiltration sensitivity run using TOUGH2 was performed, a one-dimensional steady-state equilibrium run was conducted. The purpose of the equilibrium run was to establish the initial conditions for the transient simulations. Key input parameters for this equilibrium run included:

- The upper boundary had a constant infiltration rate of 3.6 mm/yr (7.76×10^{-4} kg/s). This was the infiltration rate used in the LBNL site-scale model at the location of SD-9.

- The water was introduced into the top fracture domain.

- The lower boundary of the model was set to water-table conditions (pressure=0.91 $\times 10^5$ Pa).

- LBNL properties (DTN: LB971100001254.002) for the location of borehole SD-9 were used in the input file.

- The total simulation time was 1 million years to ensure steady-state conditions were achieved.

Results of Initial Steady-State Equilibrium Simulation

At the end of the 1-million-year simulation period, the liquid-flow rate into the top of the model was equal to the flow rate out of the lower boundary, indicating that a simulated steady-state condition had been reached with the assumed boundary conditions and model parameters. As a further check of the appropriateness of these results, SD-9 field core-saturation (matrix) measurements were plotted by elevation, along with the simulated saturation values obtained for each of the fracture and matrix elements (Figure 2-22). The figure indicates that matrix saturations agree well with SD-9 core measurements. This agreement increases confidence that the equilibrium simulation has established the appropriate initial conditions in the model. Simulated fracture element saturations are also shown in Figure 2-22. Fracture-saturation values were generally 12 to 13% or lower at elevations between 1,290 m and about 875 m. Fracture saturation values increased to 25–30% between about 875 m and about 750 m. Table 2-17 shows liquid flow in selected fracture connections as a percentage of total liquid flow in those connections at the end of the equilibrium simulation. The repository is located in the vicinity of connection 9. The initial-conditions portion (INCON) of the SAVE file (output from TOUGH2) from this equilibrium run was substituted into the input deck for the subsequent transient run.

Transient-Infiltration Simulation Parameters

The transient-infiltration simulation was performed with the same basic input deck used in the initial steady-state equilibrium simulation. The primary differences were as follows:

- Infiltration rate was allowed to vary annually for each of the first 100 years of the simulation

- Initial conditions were taken from the initial equilibrium simulation

- Total simulation time in the transient run was 100,000 years.

The transient simulation was performed using modeled infiltration rates from the USGS model (DTN: SNT05091597001.006). The USGS model was set to simulate daily conditions for 100 years, assuming the average annual infiltration rate remained at 3.6 mm/yr. Before they were entered into the input file, the daily infiltration values were summed to obtain annual total infiltration values for each of the first 100 years. From 100 years to the end of the simulation at 100,000 years, the infiltration rate was set to a constant 3.6 mm/yr. In the transient simulation, the liquid-flow rates between selected element connections were recorded at each time step during the simulation.

Summary of Transient-Infiltration Simulation Results

The results of the transient-infiltration simulation are presented in Figure 2-23 which shows normalized (to the steady-state infiltration rate of 3.6 mm/yr) liquid-flow values versus time in years. Both fracture and matrix contributions to liquid flow were summed together for the plots. The normalized liquid-flow is shown for only three of the ten original selected connections (connections 1, 4, and 9). The first connection is between the top two layers, TCw1 and TCw2. The fourth connection represents that between layers PTn1 and PTn2. The ninth connection is located approximately at the depth of the repository and represents the connection between layers TSw4 and TSw5.

As expected, the liquid flow rate in connection 1 changed quickly from the steady-state value (normalized value of 1 equals the steady-state infiltration rate of 3.6 mm/yr) in response to the transient infiltration. As indicated in Table 2-17, most of the flow in the Tiva Canyon Formation (three upper layers) was occurring in the fractures. As the water moved downward and into the Paintbrush Formation, the water imbibed into the matrix (substantially decreasing the amount of fracture flow) which slowed the movement of water through these layers. This was seen in connection 4 as a dampened change in liquid flow from the steady-state value compared to connection 1. By the time the water reached the repository horizon, the impact of transient infiltration was very minor (ranging from more than 0.99 to about 1.01), and the TSw4 to TSw5 curve is almost unchanged from the steady-state value. The maximum increase in liquid flow at the repository horizon was a normalized value of 1.0135 at 209.8 years after the start of the simulation.

As a result, the behavior of transient infiltration (evaluated every year) was not expected to be significantly different from the steady-state infiltration simulations at the repository horizon. To strengthen this assertion, future analyses should consider seasonal, monthly, or even daily infiltration variations to determine if the flux at the repository is affected by transient infiltrations that are averaged over shorter durations.

2.4.2.9 Estimation of Net Infiltration from Temperature Data

Temperature data from Yucca Mountain boreholes were analyzed by Bodvarsson et al. (1997, Chapter 11) in terms of percolation flux rates and overall heat flux. Two multi-layer analytical solutions were derived for the determination of percolation flux from temperature data, one with a constant-temperature lower boundary condition and the other with a constant-heat-flux boundary condition. The accuracy of these solutions was verified with the numerical code TOUGH2. The results of the analysis yielded percolation fluxes in the range of 1 to 10 mm/yr for most of the deep boreholes. The analytical solutions did not allow for accurate determination of percolation flux for the shallower boreholes as there was large gas flow in the shallow system, which altered the temperature profiles. Major faults may also have had significant gas flow, as suggested by temperatures from various boreholes. As a result of these analyses and other studies in Bodvarsson et al. (1997, Chapter 11), LBNL recommended an upper bound for the net present-day infiltration to be three times the mean infiltration.

2.4.3 Unsaturated Zone Flow

The preferred abstraction approach for UZ flow was simply to use the LBNL process model (Bodvarsson et al. 1997, Chapter 24) directly (i.e., no abstraction). It was initially expected that the model would be simplified, probably by reduction to two-dimensional or even one-dimensional. However, the process modelers and site-characterization data gatherers strongly recommended that three-dimensional was important to represent Yucca Mountain flow adequately. This recommendation was based primarily on the flow below the potential repository, where there is thought to be significant nonvertical flow because of heterogeneity in the locations of the zeolitic layers and perched water. With the direct use of the LBNL flow model, there is no need for testing of abstractions against the process model. The models are tested directly against the data as part of the calibration procedure (i.e., each case must be calibrated).

An important consequence of using a complex three-dimensional flow model is that the number of different cases that can be run is limited by computer-processing time, but even more so by the time needed for analysts to make necessary adjustments by hand for each case (to ensure proper model calibration). However, the current approach uses several select conceptual models and parameter sets that were determined (by sensitivity analyses) to have a significant impact on performance in order to encompass the range of uncertainty in UZ flow. Section 2.5.1 and Section 2.6.1 provide results and indicate that aqueous travel times between the repository and water table can vary by several orders of magnitude between different conceptual models.

The three-dimensional LBNL flow model inherently contains several specific assumptions and issues that are listed below:

- Dual-permeability flow modeling (i.e., coupled matrix and fracture continua) is adequate. The DKM is capable of representing a large range of potential UZ-flow behaviors (e.g., fracture-matrix interaction, fracture and flow-channel spacing and geometry, effective fracture apertures, and fracture- and matrix-flow velocities all vary greatly as the model parameters vary). In future work, alternative models of the sort discussed in Chapter 24 of Bodvarsson et al. (1997) (e.g., discrete fractures, fractal fractures, etc.) can be used to complement dual-permeability models, but they were not considered for TSPA-VA.

- Steady-state flow modeling is adequate. Climate changes have been included by using a series of steady states; because of that, the flow could be said to be quasi-steady state rather than steady state. Perturbations to flow caused by repository heating were neglected. Such thermohydrologic perturbations were considered only in sensitivity cases because the waste packages are expected to last through the period when flow is strongly perturbed (refer to Section 2.4: Thermal Hydrology).

- Hydraulic properties of the matrix can be represented by the range of laboratory measurements. In some cases matrix properties were adjusted to get better fits to matrix-saturation measurements or other data (see Section 2.4.3.1.3 and Section 2.4.3.1.4 for details).

- Fracture hydraulic properties can be derived from air permeabilities, fracture frequencies, and fracture orientations measured in drill holes and in the ESF. In some cases, the inferred fracture properties (van Genuchten alpha) were adjusted significantly in order to get better fits to matrix-saturation measurements or other data (see Section 2.4.3.1.3 and Section 2.4.3.1.4 for details).

- The van Genuchten/Mualem functional form is satisfactory for use to represent the saturation/desaturation behavior of both matrix and fractures.

- The fracture-matrix connection area (i.e., area available for flow between fractures and matrix) is reduced below the geometric area implied by the fracture spacings used. Physically, this reduction represents effects of channelization of flow in fractures. The amount of reduction was chosen to optimize the fit to matrix-saturation measurements or other data.

- Heterogeneity within a unit does not need to be included (hydrogeologic units are homogeneous).

- Infiltration at the surface is spatially variable, with the variability given by data in Flint et al. (1996). Sensitivity to infiltration was investigated by multiplying the infiltration distribution by a constant factor, keeping the same spatial variability.

- The lower boundary of the model is at the water table, which is fixed by drill-hole observations. For future climates, the water-table elevation increased by prescribed amounts as described in Section 2.4.1.1.

The following sections address many of the above assumptions and relevant UZ flow issues (see Table 2-4) through sensitivity analyses or calibration studies. A number of these analyses were performed by Bodvarsson et al. (1997) in the development of the three-dimensional LBNL UZ flow model and are simply summarized below.

2.4.3.1 Hydrologic Properties and Calibration

The LBNL UZ flow model characterizes the large-scale hydrogeologic and geologic heterogeneities in the UZ at Yucca Mountain. It incorporates many of the geological complexities found in the UZ, including stratigraphy, faults and associated offsets, dipping beds, and zones of alteration. Table 2-18 shows the relationship between geologic formations and model layers in the LBNL UZ flow model. By incorporating geologic and hydrogeologic complexities it is able to fulfill one of its roles, which is to provide a baseline description of the ambient hydrologic state of the UZ. Calibration against measured data is a critical step in the development of the UZ model to represent ambient conditions. The available measurements characterizing ambient conditions in the UZ at Yucca Mountain consist of the following:

A. Core sample saturation and water potential data (Flint 1998, pp. 40-43, 48-53)

B. Geophysical saturation data (Thompson and Rael 1996, pp. 1-24)

C. Core sample porosity and rock grain density data (Flint 1998)

D. In-situ water potential and temperature measurements (Rousseau et al. 1998)

E. Layer-averaged matrix permeability and van Genuchten parameters from core sample measurements (Flint 1998, pp. 21-29)

F. Layer-averaged fracture parameters such as permeabilities (from in situ tests) and van Genuchten parameters developed through LBNL analyses (LeCain, 1997, pp. 4-32; Ahlers et al. 1996)

G. Spatially varying infiltration rates (Flint et al. 1996)

H. In situ pneumatic data (Rousseau et al. 1998)

I. Geochemistry data such as chlorides used to check travel-time predictions (Table 2-1).

The saturation and water-potential data depict the ambient hydrologic state of the UZ at Yucca Mountain. The primary use of these data in a calibration effort is to develop a set of hydrogeologic parameters that will allow the model to simulate the ambient condition. However, since the saturation and water-potential data are available for relatively few boreholes, the calibration effort is assisted by using input parameter values measured in core samples collected during drilling. The next sections discuss how matrix and fracture parameters are determined for use in the calibration procedure.

2.4.3.1.1 Matrix Permeability and van Genuchten Parameters

Numerous core sample measurements have been performed in the past in order to calculate permeability and van Genuchten model fitting parameters. The USGS has provided the Q results of matrix property analyses on borehole core samples that give geologic-layer mean values and uncertainties (Flint 1998, pp. 32-46) The data set includes saturated hydraulic conductivity, van Genuchten fitting coefficients (van Genuchten 1980, pp. 892-898), and residual saturation for a number of boreholes. In this section, matrix van Genuchten model coefficients are referred to as matrix alpha (α) and matrix m (Ma and Mm, respectively), while fracture coefficients are referred to as Fa and Fm.

The van Genuchten fitting coefficients are calculated by combining the results from separate desaturation-curve measurements on core samples and fitting a curve using the van Genuchten model through the combined data set. In some cases, available saturation and potential measurements on core samples obtained during drilling are used to increase the number of data points used in the curve fit. The matrix alpha (Ma) and matrix m (Mm) values estimated through this process are affected by the resolution of the measurement instrument. The potential measurement resolution is about 1.3 bars for nearly saturated samples, with an error of 100%. The absolute error increases at more negative (drier) potentials, although the percent error is smaller. The variation in data accuracy may affect the results of the curve-fit standard error calculation.

The combination of the data from separate desaturation-curve measurements on different samples into one data set provides a significant reduction in the standard error of the curve fit. For example, converting the data for model layer tsw34 (Tptpmn) to log10 values, the alpha value reported by Flint (1998, p. 45) from the combined data-set-curve fit is about -6.2 ± 0.08 (standard error of 0.08). However, if a curve is fit to one of the individual data sets, the results of the curve fit provide an alpha of -6.3 ± 1.17. The individual data-set fit has a log standard error more than an order of magnitude higher than the standard error from the combined data-set fit.

Flint (1998, p. 44) reports mean, saturated hydraulic conductivities (Ksat) for selected hydrogeologic formations with three different averaging methods: arithmetic, geometric, and power law averaging. Furthermore, the USGS reports that there were a number of core samples for which conductivities were too small to be measured with the available test apparatus. These "nondetect" values were not included in the final averages (Flint 1998, p. 39). An alternative approach is to determine the smallest Ksat that can be measured with the test equipment and use that value in the mean calculations in layers where nondetect values are reported. By incorporating the nondetect values, a significant number of the layers have reduced mean conductivities, some by more than an order of magnitude. The standard deviations would also generally increase, although in layer tmn there are so many nondetect values that the standard deviation would decrease along with the mean conductivity. The "nondetect" values for matrix hydraulic conductivity are primarily in welded units where flow is predicted to be partitioned almost entirely in the fractures. The inclusion of very small "nondetect" matrix permeabilities in these units is not expected to alter the percolation distribution significantly. The impact of neglecting these "nondetect" hydraulic conductivities is considered in Section 2.6.1.3, where sensitivity analyses are conducted by increasing and decreasing the permeability of the zeolitic matrix units. Results indicate that a decreased permeability (by one standard deviation) of the zeolitic matrix does not affect travel times appreciably, and the impact on overall performance is not expected to be significant.

2.4.3.1.2 Fracture-Hydrogeologic Parameters

A consistent set of fracture properties was developed for the LBNL UZ flow model using fracture data from the ESF and borehole measurements (Bodvarsson et al. 1997, Chapter 7). The Detailed Line Survey ([DLS]: performed by the USGS/Bureau of Reclamation) provided a systematic set of fracture locations, trace lengths, and orientations in the ESF, from which both average and spatially varying properties were obtained. Using mean fracture permeabilities derived from air-injection testing (LeCain 1997, pp. 4-32) and fracture frequencies and intensities calculated from borehole data (Rautman and Engstrom 1996, pp. 22-26) and the DLS, a set of mean hydraulic fracture apertures and fracture porosities was determined for intervals corresponding to the LBNL flow model layers. Combining air-injection permeability measurements performed at a range of spatial scales in the Topopah Spring middle nonlithophysal unit (LeCain 1997, pp. 4-32) allowed for an estimate of the fracture aperture distribution. From this distribution an analytical solution gave the capillary pressure vs. saturation curve from which van Genuchten parameters were obtained.

In previous versions of the UZ model before October 1996, all model layers were assigned fractures except the layers corresponding to the PTn. The bedded layers, in particular, were expected to prevent the propagation of fractures. However, since significant numbers of fractures are observed and reported in the ESF for the layers that comprise the PTn, the current UZ-flow model was developed with fractures in all units, using the DKM representation of the UZ.

The DLS gives the position of fractures along the ESF, their lengths above and below this line, the strike, dip, and various other observations. In a large part of the ESF, fractures down to a trace length of 0.3 m were measured, yet after the middle nonlithophysal unit of the Topopah Spring had been partially mapped, a minimum trace length of 1.0 m was imposed (Beason 1996, pp. 7-9). The work by Bodvarsson et al. (1997, Chapter 7) included data up to Station 40+00 (see Figure 2-24 for sketch of the ESF). Additional data from the main drift and south ramp can be considered in future work for a more complete compilation of mean properties and spatial variations in fracture properties.

The following sections deal with the development of fracture properties for the LBNL UZ site-scale model layers. These have all been calculated from the "raw" data presented in the DLS, borehole measurements, and air-injection tests. In this way, the data are consistent with the most recent implementation of the Geological Framework Model implementation into the UZ site-scale model.

Fracture Frequencies, Intensities, and Lengths Calculated From the DLS Data

Based on geologic descriptions of the units, intervals along the ESF were assigned to the different UZ model hydrogeological units. All model layers were described in Bodvarsson and Bandurraga (1996; Chapter 2) and in Bodvarsson et al. (1997; Chapter 3). Although the data set extended to Station 40+00 (4,000 m), the region between Stations 35+00 and 40+00 were not included in the compilation of mean properties because this section of the ESF included the Sundance Fault and a region of unusually low fracture density north of the Broken Limb Fracture Zone. In order to obtain a consistent set of fracture frequencies, trace lengths less than 1 m were not included in the averages. Fracture frequencies determined from the DLS measurements were not corrected for any possible bias in orientation. The effect of excluding fractures with a length less than 1 m is that the reported fracture frequencies might be less than if smaller fractures were included. This, in turn, would reduce the predicted fracture porosities and increase the predicted fracture apertures. Porosities are not part of the steady-state governing equations for UZ flow, so variations in porosity would not affect the UZ-flow results. Fracture apertures are used to estimate fracture van Genuchten air entry values (α_f), and larger apertures would lead to increased fracture van Genuchten air entry values. However, as shown in Section 2.5.1.3, the travel times are not sensitive to variations in van Genuchten air entry values.

Mean fracture spacing and frequency were determined in Bodvarsson et al. (1997; Chapter 7). In addition to the average spacing and the frequency for each interval, the fracture intensity, I (m/m^2) was calculated using the sum of the trace fracture trace lengths in a given interval, over an approximate area of the ESF enclosing the fractures. A 3-m high band above and below the centerline of the DLS was chosen because it encompasses an area that includes most of the fractures. It was assumed that the few fractures that extend outside this band were offset by many smaller fractures that do not cross the centerline, yet may be enclosed in this region.

Fracture Frequencies from Borehole Measurements

Measurements of fracture frequencies from core samples were used for units in which ESF data do not exist (i.e., the unit was not encountered) (Bodvarsson et al. 1997, Chapter 7). Because it was impossible to distinguish between small fractures on the order of tens of centimeters and those several meters or greater in diameter, borehole fracture frequencies were much higher than those measured in the ESF, where a minimum size of 0.3 m was enforced. For compatibility with the ESF measurements, several corrections were made to the data. First, only the fractures that were designated natural or indeterminate (N+I) were chosen, and the number of fractures per ten-foot interval were then corrected by the proportion of core that was lost or retrieved as rubble. In the borehole data that were examined, the number of fractures per interval were given for three ranges of fracture dip orientations (0–30, 30–60, and 60–90 degrees), and each set was corrected. The second correction was made for the bias of horizontal fractures in a vertical borehole using the relation in Altman et al. (1996).

In comparison to fracture frequencies in the ESF, for fractures at least 1 m in length, the borehole frequencies are nearly an order of magnitude higher. In the ESF, the proportion of fractures having trace lengths between 0.3 m and 1 m may be 50% or greater. Because of the approximately lognormal distribution of fracture lengths, a large proportion of fractures that are less than 0.3 m in length would also exist in the boreholes. Therefore, in order for the borehole frequencies to be compatible with those compiled from ESF measurements, which were tabulated for fractures 1 m or greater in length, a correction must be made to the borehole data. A simple method is to assume that the ratio between the fracture density for a layer in the borehole and the ESF is about the same for all layers. A large quantity of data was collected from the ESF and in boreholes for the three reference model layers TSw32, TSw33, and TSw34 (see Table 7.8 in Bodvarsson et al. (1997).

Fracture data for the Calico Hills and the lowermost Topopah Springs unit (Calico Hills vitric unit [CH1vc] or Calico Hills zeolitic unit [CH1zc]) were provided from the qualified Boreholes SD-12 and NRG-7A (Rautman and Engstrom 1996, pp. 11-13, 22-26). Corrected frequencies for Borehole SD-12 were quite similar for the reference frequencies TSw32, TSw33, and TSw34, giving confidence in this simple approach. A small section of the zeolitic layer of the Calico Hills had no measured fractures, but was included because it was part of the original data set.

Corrected fracture frequencies for the TSw and CH1vc units in NRG-7A differ little from SD-12 and the ESF. The lowermost few feet of NRG-7A has high saturations, indicating that it should correspond to the zeolitic layer CH3zc, even though the fracture frequency is unusually high. This sample is represented by only a few feet at the bottom of the core; therefore, the data may be unreliable. Hence, no calculations were performed using frequencies from this measurement.

Fracture Permeabilities from Air-Injection Tests

Permeabilities obtained by air-injection tests in boreholes are believed to be representative of the fracture permeability (LeCain 1997, pp. 4-32). Mean values of the fracture permeabilities for the LBNL UZ model hydrogeological units were calculated from the individual air-injection permeabilities given by LeCain (1997) from Boreholes SD-12, UZ-16, NRG-6, and NRG-7a.

Air-injection permeabilities from vertical boreholes are biased toward the horizontal permeability. Because near-vertical fractures dominate the large-scale air permeability at Yucca Mountain (Ahlers et al. 1996), the vertical permeability is expected to be larger. This has also recently been noted by LeCain (1997); permeabilities from pneumatic-monitoring in the Topopah Spring Tuff are an order of magnitude higher than values obtained from air-injection, indicating a ten-times-higher vertical permeability compared to the horizontal permeability. Pneumatic-monitoring and air-injection permeabilities were shown to be comparable for the Tiva Canyon tuff and Paintbrush nonwelded tuffs (LeCain 1997).

Ideally, the fracture frequency and the fracture permeability should show some correlation. An increase in fracture frequency may, in addition to increasing the permeability by the greater number of pathways, also lead to increased connectivity. A comparison between the fracture frequency and the air-injection permeability (log k) shows only a slight overall positive correlation. The one zeolitic sample, though, does have a significantly lower fracture frequency and permeability, but the samples from other units show significant scatter. Connectivity and possibly fracture aperture may, however, dominate the air permeability at the scale of these measurements (approximately 4- to 10-m packer intervals). No relationship between the fracture intensity and the fracture permeability was found (Bodvarsson et al. 1997, Chapter 7).

Fracture Apertures

Although some rough measurements of fracture apertures were made for the DLS, the large-scale effective aperture for flow is impossible to measure in this way. Therefore, estimates of fracture aperture require (1) a large-scale permeability (e.g., one obtained from air-injection testing); (2) an assumption that the fractures are fully connected; and (3) an equation for the velocity within a fracture. Assuming that the velocity within a fracture is given by the cubic law (Domenico and Schwartz 1990, pp. 86-87), the fracture aperture, b, can be obtained from the air permeability (k) and the mean fracture frequency.

It is assumed that the air permeability is equivalent to the fracture permeability. This is likely to be a good approximation in the highly fractured welded units having low matrix permeabilities and high matrix saturations. In the PTn bedded tuffs, with their higher matrix permeabilities and fewer fractures, the fracture permeability is probably overestimated. Average fracture frequencies calculated from the ESF data and from borehole data were used to calculate apertures. Layer TCw11, and the vitrophyres TSw31 and TSw37, did not have permeability measurements. The Calico Hills vitric unit also did not have an air-permeability measurement; it was calculated by assuming an aperture of 170 μm, based on the apertures of 171 and 165 μm used in the adjacent units.

Van Genuchten Parameters for Fractures

The van Genuchten equation for relating effective saturation to capillary pressure is used to govern unsaturated flow through fractures, where α and m are fitting parameters (van Genuchten 1980, pp. 892-898). Assuming the simplified form of the Young-Laplace equation, as was done by Altman et al. (1996, pp. 43-44), values of α (Pa^{-1}) may be calculated directly from the fracture aperture b (mm).

Alternatively, to obtain m and α, a curve of P_c versus liquid saturation must be generated based on a known or derived aperture distribution. The best fit then yields m and α. Several fundamental assumptions must be made for the estimation of the mean fracture aperture, the aperture size distribution, and the van Genuchten parameters relating liquid saturation to capillary pressure. The first assumption was that the air-injection permeability measurements from boreholes (LeCain 1997) and those taken in drifts off the ESF (Bodvarsson et al. 1997, Chapter 7) represent the permeability distribution of the fracture system. Second, it is assumed that the large-scale fracture permeability (k) can be approximated by the parallel-plate assumption (cubic law as presented in Domenico and Schwartz, 1990, pp. 86-87).

The mean fracture permeability is given by the geometric mean of all measurements in a given hydrogeologic unit, in this case the Tptpmn. The mean fracture frequency is given by the average of the inverse of the linear fracture spacings calculated from the DLS measurements performed in the ESF. There are some flaws in this characterization. First, the permeability measurements are likely to be more related to the connectivity of the fractures than to their individual permeabilities. Second, given that the connectivity may dominate the system, the permeability variations are not directly a function of the aperture distribution within a single fracture. However, the aperture variation within a single fracture is unlikely to represent the full variation in apertures of all fractures, given the log-linear nature of the trace length distribution. Experimental studies on single fractures (e.g., Reitsma and Kueper 1994, pp. 865-878), along with other estimations of aperture distributions (Kwicklis and Healy 1993, pp. 4091-4102; Wilson et al. 1994, Chapter 12, pp. 1-24), have given quite narrow distributions. From measurements in the ESF it is evident that fracture apertures vary from up to several mm down to near zero (cemented), and it is likely that larger fractures exhibit a broader distribution than do smaller ones.

A mean aperture of about 81 μm was calculated from the ESF borehole frequencies and the combined air permeability measurements for the Tptpmn (TSw34). An analytical solution (Bodvarsson et al. 1997, Chapter 10) yields the fracture capillary-pressure curve. A nonlinear least-squares fit to this curve was performed. This fit yielded an m-value of 0.633 and an alpha value of 1.274×10^{-3} Pa^{-1}. This alpha value is slightly larger than that calculated directly for the TSw34 model layer (9.73×10^{-4} Pa^{-1}), which used solely the larger-scale air permeability measurements by LeCain (1997, pp. 23-27). The m-value compares favorably with that of Kwicklis and Healy (1993, pp. 4091-4102), and Wilson et al. (1994, Chapter 12, pp. 1-24). Measurements in natural fractures (Reitsma and Kueper 1994, pp. 865-878) are even higher, indicating a narrower aperture range.

Fracture Porosity

The fracture porosity is important for modeling liquid and chemical fluxes between fractures and matrix. The fracture porosity is calculated in one, two, and three dimensions, with assumptions as to the fracture aperture, connectivity, and geometry (see Chapter 7 in Bodvarsson et al. (1997) for more details).

Fracture porosities can be estimated in three dimensions by assuming a fracture shape (e.g., circular disks) and expressing the porosity as the total volume of fractures per rock volume. The three-dimensional porosity can then be obtained by dividing the total fracture volume by the rock volume enclosing the fracture disks. First, the area of the ESF enclosing the fracture traces must be estimated, which is uncertain because long fractures extend into areas where smaller fractures do not cross the centerline and therefore were not included. An area was chosen with dimensions that extend past the extent of most of the fractures, but not so large as to include large areas where fracture traces were not measured. The area enclosed by the fracture traces was approximated as a 3-m band on each side of the centerline of the DLS (as in the calculation of fracture intensity). In general, the few fractures that extend well past this area are assumed to be balanced by the somewhat larger area that is chosen surrounding the fracture traces. For the three-dimensional porosity, the depth of the rock volume was approximated to equal the height (6 m).

Fracture porosities can be estimated in two dimensions from apertures and total fracture length per area (fracture intensity). A two-dimensional porosity is calculated simply as the total fracture area (aperture times trace length) divided by the area enclosing the traces.

Fracture porosities calculated by the three-dimensional method are intuitively the best approximation. However, because the apertures are calculated by assuming continuous fractures, the three-dimensional method may underestimate the porosity, because a discrete fracture network may require larger apertures for the same large-scale permeability. Another reason for the three-dimensional calculation leading to an underestimate of the fracture porosity is that it assumes that the fracture traces represent the diameters of fractures, which underestimates the true fracture diameters. Therefore, in the site-scale UZ model, the two-dimensional porosities are used for the units exposed in the ESF, and one-dimensional porosities are derived from boreholes for the underlying layers. The one-dimensional porosities are calculated as the fracture aperture divided by the fracture spacing, assuming parallel one-dimensional fractures.

Faults

Faults are important to an understanding not only of the ambient conditions at Yucca Mountain but also of the performance of the mountain as a geologic repository for high-level nuclear waste. Faults have been shown to act as "fast" or preferential pathways for conducting transient pneumatic signals (Ahlers et al. 1996). They may act as drains for surface infiltration that exceeds the conductive capacity of the welded units. It is not understood whether faults act as (1) capillary barriers to lateral flow of moisture because of increased fracturing and drying resulting from gas flow, or (2) as permeability barriers because of fault gouge, or (3) both. On the other hand, they may not act as barriers to lateral flow at all. With waste emplacement and subsequent heating, they may become chimneys through which heated air and water vapor escape to the surface.

The number and type of faults at Yucca Mountain are fairly well understood. However, not enough data exist to determine whether faults have similar pneumatic/hydraulic properties, or whether each type of fault or part of a fault (e.g., those with brecciation, gouge, etc.) has similar properties (Chapter 7 in Bodvarsson et al. 1997).

The ambient pneumatic pressure data can be used to estimate pneumatic diffusivity of the fracture continuum in the faults. With the addition of fracture-continuum permeability from air-injection tests and fracture-intensity data, permeability and porosity of the fracture continuum can be estimated. In some units the porosity of the matrix contributes to the pneumatic diffusivity of the fault.

Ambient pneumatic-pressure data have been used to estimate pneumatic diffusivity of faults in the TCw, PTn, and TSw. There are no pneumatic pressure data from fault zones below the bottom of the TSw, so no estimates of these parameters are available. Ahlers et al. (1996) describe parameter estimation using the UZ site-scale model. Pneumatic diffusivity is estimated for each of four faults: the Ghost Dance Fault, the Drill Hole Wash Fault, the Bow Ridge Fault, and the unnamed, north-trending fault connecting the North Ramp of the ESF and the area near Boreholes UZ #4 and UZ #5.

Air injection testing in GTB #1 provides estimates of pneumatic permeability in the middle nonlithophysal zone of the Topopah Spring Tuff. Figure 7.7 in Bodvarsson et al. (1997) shows eight values of permeability that range from a minimum of 1.3×10^{-12} m^2 to a maximum of 11.1×10^{-12} m^2, with a mean value of 5.5×10^{-12} m^2.

If all faults in the site-scale model area are grouped together, then an average permeability can be calculated for each of the hydrogeologic units in the faults. The standard deviation of the PTn fault permeability is the lowest. This is consistent with other estimates of pneumatic permeability, as estimates for the PTn are generally best constrained by the pneumatic data.

2.4.3.1.3 Calibration Approach

This section contains a summary of the calibration approach used to develop hydrologic parameters for use in the site-scale UZ-flow model. A more detailed description of the methods and approach can be found in Bodvarsson et al. (1997, Chapter 6).

Typical parameter sets estimated in calibration against moisture and gas flow data consist of the permeability and van Genuchten fitting coefficients for both matrix and fractures. Residual saturations can also be estimated in the calibration, but have been shown in past calibration efforts (Bodvarsson and Bandurraga 1996) to be relatively insensitive compared to the other parameters. Since the fracture-data uncertainties are much higher than those of the matrix properties, the emphasis has been to honor the reported matrix data as much as possible in the calibration efforts. Also, attempts have been made to reduce the number of parameters estimated in the calibration by coupling permeability and van Genuchten alpha parameters, using theoretical relationships and regression equations based on measured data (Bodvarsson and Bandurraga 1996). However, the coupled approach has not been successful, as discussed in those reports. Therefore, the current calibration effort is focused on separately estimating the permeability and van Genuchten parameter set for both matrix and fractures.

The general approach to the calibration effort involves a number of steps. First, a number of vertical one-dimensional submodels are developed from the full three-dimensional model corresponding to the borehole locations selected for use in the calibration of moisture flow. The submodels share discretization, zonation, and boundary conditions such as infiltration rates with the full three-dimensional UZ model. The submodels are used in a simultaneous inversion with measured saturation and water potential data to estimate a layer-averaged parameter set. Available pneumatic data are then used in another simultaneous inversion to revise only the layer-averaged parameter set fracture permeabilities to match borehole gas pressure records. Next, data from each borehole selected for use in the calibration are matched during an individual inversion to evaluate the spatial variation in each parameter across the model domain. The results of all of the one-dimensional submodel inversions are evaluated based on the following criteria:

- Are the saturation and water potential data matched?
- Are the resultant inversion parameters consistent with the variances provided by the parameter measurements on core samples?
- Does the resultant alpha parameter set provide fracture alphas that are larger than the matrix alphas? Because alpha is inversely related to capillary pressure, one would expect that fractures should have a larger alpha.
- Are the alphas for layers within a hydrogeologic unit consistent throughout the unit?
- Are the fracture/matrix mass fluxes and travel times within a model layer consistent with the conceptual model of flow as determined based on geochemical data such as chloride concentration in bodies of perched water and locations of bomb-pulse ^{36}Cl occurrences?

Once a base-case parameter set is established based on these criteria, various inversions using different modeling approaches and infiltration rates are performed to evaluate the sensitivity of the results to these factors.

Submodel Development

The submodel used in the moisture-flow calibration consisted of more than 20 layers in each one-dimensional column, depending on the height of the column above the water table. Each model layer had a set of initial property estimates for the matrix and fractures, including relative permeability and capillary-pressure functions. The boundary conditions for the one-dimensional columns are set as follows: at the top, the columns are open to the atmospheric conditions but act as no-flow boundary to liquid, and a constant temperature of 25°C is applied. The appropriate mass flux calculated from the infiltration rate is applied to the top TCw layer of each one-dimensional column in the model. Since the TCw is densely welded and highly fractured, mass flux is introduced in the block representing the fractures (for DKM). The gas pressure at the water table is held constant at about 92 kPa. A steady-state calculation is performed using the EOS3 module of TOUGH2.

The inversion code that performed the calibration was the ITOUGH2 program (Finsterle 1993, pp. 1-23). The appropriateness of fit of the calibration is measured using the standard least squares approach, which minimizes the sum of the squared residuals weighted by the inverse standard deviations of the data. The water potential and saturation data measured in each layer were averaged and standard deviations calculated. An arithmetic average is used for the saturation data, and a geometric mean is used for the water potential data.

The effect of using average values to represent the sometimes widely scattered data available from borehole core-sample measurements is shown in Figure 6.3.1-1 of Bodvarsson et al. (1997, p. 6.19) with the data from Borehole SD-9. The plot shows the reported USGS saturation and water-potential data, as well as the average values and standard deviations calculated for each layer used in the model calibration as match points. The averages calculated for the potential data have excluded data less than -30 bars, as discussed earlier. The data are widely variable, even within a relatively homogenous geologic formation. The relatively low, average, matrix saturation calculated for the model layer corresponding to the basal vitrophyre is somewhat surprising, given the existence of perched water above the vitrophyre. However, the matrix saturations in the layers underlying the vitrophyre may have some effect on the data. Also, if the perching occurs on top of the vitrophyre, with a low matrix permeability resulting from extensive zeolitic alteration in the fractures, perhaps there is significant lateral diversion, so that vertical flow through the vitrophyre is much less than vertical flow above it. There is also the difficulty associated with measuring saturations and potentials in the extremely low-porosity (average 2%) vitrophyre layer. Any sample disturbance during drilling and handling could have a significant effect on the measurements.

Calibration Assumptions and Issues

The approach used during the moisture flow portion of the calibration is based on a number of assumptions, including the following:

1. **Steady-state conditions**. The calibration assumes that saturation- and water-potential data represent the hydrologic state of the UZ under steady-state conditions and constant infiltration rates. This is consistent with the fact that changes in net infiltration through the matrix are expected to occur gradually over thousands of years as a result of climate changes. However, the relatively slow travel time through densely welded portions of the matrix makes it possible that saturations at depth within the mountain actually are a reflection of historic conditions with much different infiltration rates. The steady-state assumption is consistent with the fact that any resultant infiltration pulses that occur may be attenuated by the redistribution of moisture via, and evaporation into, the air moving through the mountain as a result of barometric pumping (Weeks 1987, pp. 165-170). Also, modeling studies in Section 2.4.2.8 have shown that the PTn serves to attenuate yearly infiltration pulses, creating near-steady-state conditions in the TSw.

2. **Validity of the DKM for UZ flow process simulation**. Previous UZ modeling work at LBNL has mainly used the ECM approximation, although DKMs were incorporated into the fiscal year (FY)-96 milestone report (Bodvarsson and Bandurraga 1996) and have been used in the calibrations performed by Bodvarsson et al. (1997). Studies by Bodvarsson and Bandurraga (1996, Chapter 6) showed that the DKM provided better simulations of transient and thermally perturbed UZ processes and transport. Therefore, the DKM formulation is used for a majority of the moisture and gas-flow calibration work. Parameter sets based on the ECM formulation will continue to be provided to the project, as these are used for TH studies.

3. **Validity of the van Genuchten model for the relationships between water potentials and saturations in the matrix and fractures and liquid relative permeabilities**. In the

absence of reliable data of the relationship between saturation and relative permeability for welded and nonwelded tuffs, the van Genuchten model is used for both fractures and matrix in the UZ model.

4. **Validity of pneumatic permeability data for liquid-flow properties through the fracture**. The air-k tests and pneumatic analyses provide measures of permeability for the fracture systems.

A number of issues must be addressed when developing the calibration methodology. The following paragraphs examine some of the modeling issues evaluated before performing the study.

Comparison of Field Data to Model Results

Conceptual and numerical differences exist between the values obtained in the field and the corresponding model variables. The most obvious differences are a result of the scaling problem. The saturation data, for example, reflect conditions on a local scale on the order of centimeters to meters, whereas the model-calculated values represent average saturations on the scale of an individual model grid block, which can be on the order of tens of meters. Since the intention of this study was to provide parameters to the full three-dimensional UZ model, the three-dimensional model discretization was used in the calibration submodels (Chapter 6 in Bodvarsson et al.1997).

Heterogeneity Scales

Another issue concerns the limit to the heterogeneity that can be resolved in a three-dimensional site-scale model. For example, boreholes UZ#4 and UZ#5 (Loskot and Hammermeister 1992, pp. 13-33), which are only about 40 m apart, show different saturation, water potential, and temperature profiles (Rousseau et al. 1998). This points out the problem of the scale of the heterogeneities that can be resolved by a site-scale model, since the smallest model gridblocks have equivalent radii on the order of tens of meters. The UZ model represents lateral and vertical heterogeneities in geologic formations at this scale, such as broad alteration transition zones, faults, and average fracturing intensity. The model is not expected to resolve heterogeneities that occur at smaller scales.

Selection of Matrix Property

The matrix properties to be used in the calibration were obtained from laboratory measurements on plugs from core samples several centimeters in diameter. Flint (1998, p. 44) has addressed the upscaling issue by presenting a number of averages for the matrix properties. The power-law average, in particular, is formulated to provide a mean value that incorporates the results of upscaling analyses by McKenna and Rautman (1996, pp. 12-13, 24-34, 70-71). However, the site-scale model, as it has generally been formulated in the past (ECM), has usually required an increase for some of the average matrix permeabilities reported for the various layers to match measured matrix saturations. Because of this, the geometric means reported by Flint (1998, p. 44) were used as the initial guesses in the calibration effort because they are somewhat higher than the power-law averages. The matrix permeabilities used as initial guesses in the calibration efforts did not incorporate the nondetect data discussed earlier. Incorporating the nondetect data has the effect of reducing the permeability averages, which is inconsistent with the results of previous calibration work.

Selection of Calibration Parameters

As discussed earlier, little is known about the van Genuchten parameters of the fracture, and field measurements are not available for calibrating the fracture properties. Because of the variances associated with the air-k data and van Genuchten fracture parameters, there has been some discussion by project personnel about attempting to lump all of the uncertainty into the fracture properties and holding the matrix properties constant during the calibration process. However, previous calibration efforts (Bodvarsson and Bandurraga 1996; Bodvarsson et al. 1997; Chapter 6) have shown that the two most sensitive parameters in matching matrix saturations and water potential data are the matrix permeability and fracture van Genuchten alpha parameter. Assuming current infiltration rates on the order of millimeters per year given by Flint et al. (1996), and using the matrix properties from Flint (1998, p. 44) and the fracture properties presented earlier, a saturated matrix is predicted for many of the model layers in the ECM formulation. This is also true for the DKM formulation, unless the interaction between the fracture and matrix blocks is significantly reduced in some way.

If the matrix permeability (Mk) is not allowed to vary during the calibration for model layers where fracture/matrix interaction is not significantly reduced, then the fracture alpha (Fa) must decrease in order to increase fracture saturations and reduce matrix saturations. The required decrease in alpha to accomplish this could cause Fa to be similar in magnitude to the measured matrix alpha (Ma) for some of the model layers. This could be true only if the predominant fracture apertures were the same size as the matrix pore sizes, a physically unreal situation. Because of this, matrix permeability was allowed to vary during the base-case inversions. The variation is constrained according to the standard deviations provided in Table 6.2.7-1 of Bodvarsson et al. (1997, p. 6.14). The residual saturations were not found to be sensitive parameters during previous calibration work and sensitivity studies (Bodvarsson and Bandurraga 1996; Altman et al. 1996, pp. 114-117) and consequently were fixed at the matrix values provided by Flint (1998, p. 18) or an assumed value of 0.01 in the fractures.

Fracture van Genuchten m Parameter

Previous calibration work (Bodvarsson and Bandurraga 1996) using the UZ model assumed the initial-layer fracture van Genuchten m parameter (Fm, where Fm=1-1/n) was equal to the matrix value. This led to Fm's ranging from 0.2 to 0.6. This assumption implies that the distribution of fracture apertures has the same log-normal standard deviation (but not the same log-normal mean) as the pore-size distribution of the matrix material. As discussed earlier, this assumption generally provides a much broader distribution of apertures than the project has thought likely during past studies (Wilson et al. 1994, Chapter 21, pp. 1-30). Because a larger m value indicates a narrower aperture distribution, with a smaller percentage of apertures that can be saturated under equilibrium with matrix water potentials, a larger m value provides a smaller fracture saturation. Preliminary calibration work indicated that a fracture m value of 0.67 in the UZ model provides fracture saturations on the order of 5% or less in the TSw model layers. A fracture m value of 0.6 is consistent with a log-normal standard deviation of the distribution of about 0.3. If the standard deviation is increased to 0.5, then the resulting m value is 0.492 from an analysis of the saturation/water potential of the fracture. This provides fracture saturations on the order of 10% in the TSw.

Little is known about fracture saturations, except for anecdotal evidence of flowing fractures in the heater test block area and wet conditions in areas of the ESF that have been isolated from communication with ventilated areas. This may indicate that some fractures or portions of fractures have relatively high saturations that are more consistent with lower m values. Wet zones have also been observed in the PTn in the South Ramp of the ESF. Flint (1998, pp. 32-39) reports that samples yielding the highest saturated-conductivity results can have some microfracturing associated with them. Although the relationship between the microfracture contribution to flow under saturated test conditions and its contribution to UZ flow is unclear, the lower m value may be consistent with the incorporation of these microfractures in the aperture distribution.

Issues with NonUnique Parameter Sets

Because of the discretization used in the UZ model and the relatively small number of available boreholes with Q data for use in the model calibration, the simultaneous calibration of moisture flow consists of inverting for as many as 151 parameters with somewhat less than 300 saturation and water-potential match points. The resultant parameter sets are not well constrained, and many sets can be obtained that would match the matrix saturations and water potentials measured at Yucca Mountain. Therefore, to reduce the nonuniqueness, the calibration results must be evaluated for consistency with physical relationships between parameters and with the conceptual model for UZ flow. In TSPA-VA, the degrees of freedom have been further reduced by prescribing hydrologic properties that have been measured; only highly uncertain parameters, such as the fracture/matrix interaction factor (see next section), are estimated using calibration methods. As discussed in Section 2.2.3, although it is possible to fit the available data with multiple calibrated models, one of the functions of PA is to consider such uncertainties and demonstrate their relation to repository performance through the evaluation of multiple conceptual models and parameter sets. These alternative models and parameter sets are considered in Section 2.4.3.9 and Section 2.6.1.

Fracture/Matrix Interaction

In the DKM, the fracture blocks interact with the matrix blocks according to the interconnected area between the two model blocks and their respective state variables. However, field data such as the locations of bomb-pulse ^{36}Cl in the ESF (Fabryka-Martin et al. 1998, pp. 93-96) indicate that it is likely that fracture flow under current climatic conditions is a localized phenomenon. Other studies have shown that fracture coatings have been found to reduce imbibition into the matrix significantly (Thoma et al. 1990). Flow fingering in fractures may also be an important phenomenon. Therefore, the calculation results providing the fracture matrix interconnection areas and the hydrogeologic parameters based on the ESF fracture mapping data cannot be used to characterize the fracture/matrix interaction using the full connection area. Simulation results, using available property data, confirm that the fractures are generally at relatively low saturation (less than in a steady-state model), so using the full area for the fracture/matrix interaction is not physically consistent.

Reduction-factor approaches that have been evaluated for use in the UZ model include the following:

- A reduction factor that reduces the fracture/matrix interconnection area by the fraction of the saturation of the upstream block in the DKM. For example, if flow occurs from fracture to matrix blocks, then the fracture saturation is used as the reduction factor. This approach was used to generate the parameter sets in Bodvarsson et al. (1997; Chapter 6).

- A constant factor (Altman et al. 1996) applied to limit interaction between matrix and fracture blocks in the DKM. The selection of the appropriate factor to use for this approach can be optimized by estimating a different factor for each layer in the calibration.

- A reduction factor calculated for each layer by dividing the vertical fracture flow by the theoretical maximum fracture flow based on air-k permeability test results.

- A reduction factor equal to the relative permeability to liquid of the upstream block in the matrix-fracture DKM layer, as outlined by Ho (1997).

When the upstream saturation was used to reduce the fracture/matrix interconnection area by Bodvarsson et al. (1997; Chapter 6), the reduction did not have a significant effect on fracture-matrix interaction. DKM simulations using this factor continued to show nearly equal water potentials in the matrix and fracture blocks representing each model layer. As in the ECM model results, the matrix saturations could be matched only by increasing matrix permeabilities significantly or decreasing fracture alphas to a physically unrealistic level.

Therefore, to ensure that the matrix properties in the model are not changed significantly from the measured core sample properties, it is necessary to reduce the fracture/matrix area significantly in the welded layers. However, preliminary simulations showed that the use of the relative-permeability-to-liquid (k_{rl}) factor in every model layer disconnected the fractures from the matrix enough to keep all of the flow in the fractures in all layers, even the nonwelded PTn. This conceptual model is similar to the Weeps model presented in Wilson et al. (1994) and will be used as part of the sensitivity analyses accompanying the base-case parameter set (Section 2.6.1.2). For the base case, a constant reduction factor is used for all the layers.

Moisture Flow Inversions

Moisture flow inversions were performed using the one-dimensional submodels to obtain initial estimates for hydrologic parameters that were then used in subsequent calibration procedures (gas pressure and perched water). The initial fracture-matrix reduction factor that was applied to the layers representing nonwelded formations in the inversions was assumed to be 0.5. The reduction factor assumed for the welded layers was 0.0005, similar to the liquid relative permeability (k_{rl}) values observed during preliminary simulations. In addition, the fracture material properties in the bottom layer of the PTn were set equal to the matrix properties in that layer. This allowed the predominantly matrix-flow in the PTn to redistribute into the fractures in the underlying TSw layer, which yielded more consistent saturations profiles with borehole measurements. Finally, some matrix alpha value standard errors were increased from the values presented in Flint (1998, p. 45) to account for the effects of combining the separate saturation curves. The increases were applied to the model layers with relatively small alpha values and estimated standard errors such as the tcw13, tsw31, tsw34, tsw36, tsw37, ch1zc, and ch4zc. The code ITOUGH2 then used an iterative procedure to estimate the desired hydrologic parameters that yielded optimal matches between simulated and observed borehole matrix saturations and moisture potentials.

Gas Pressure Calibration

After the parameter sets satisfying the criteria outlined in the calibration approach were obtained from the moisture flow inversions, they were used to calibrate the submodel to match observed gas pressures. While the moisture-flow calibration was performed with steady-state runs, the gas-model calibration required the use of transient pneumatic data. The inversions obtained a steady-state moisture-flow solution and then applied the barometric pressure signal to the top boundary during a transient simulation. This was repeated at least once for each parameter estimated during an ITOUGH2 iteration. The DKM inversions required a minimum of 20 iterations to converge to an acceptable solution, which required numerous runs with TOUGH2.

In order to minimize the calculations needed for the inversions, the gas model calibration was simplified. The simplification was devised based on the results of the moisture flow calibration. In that calibration, fracture permeabilities (Fk) were not found to greatly affect matrix saturations and were not changed significantly from their initial estimates for most of the layers. In the gas calibration, the matrix parameters and fracture van Genuchten parameters have little effect on gas flow. Because of this, it was decided to perform the gas-model calibration allowing only the Fk parameters to vary.

The two boreholes with high resolution saturation and water-potential data and numerous pneumatic pressure sensors are SD-7 and SD-12. These boreholes are also closer to the potential repository area than the other boreholes providing pneumatic data, and so are better suited for developing parameters for that area. Therefore, these two boreholes were used in the gas model calibration using the parameter set developed from the Fm=0.492 inversion. This approach was used in the calibration presented in Bodvarsson et al. (1997, Chapter 6) and yielded satisfactory results. The saturation and water-potential data were included in the calibration to ensure that the matches to the matrix data were not affected by the gas-model calibration. The bottom sensor from SD-12 was not included in this calibration because it is located beneath a reported perched water body (Wu et al. 1997), and a one-dimensional model would show only that the fracture permeabilities are very small.

The inversions were designed to input the barometric signal as a boundary condition to the top of the one-dimensional column for a simulation time of 30 days to initialize the gas pressures throughout the mountain during the transient run. The sensor data were then matched by ITOUGH2 for the subsequent 30 days. This follows the methodology outlined in Ahlers and Wu (1997, pp. 11-16). The permeability of the top boundary is set to be 100 darcies in order to propagate the pneumatic signal through the boundary without attenuation.

For much of the moisture-flow-calibration work in this study and previous efforts, the matrix relative gas permeability (k_{rg}) has been assumed to be equal to 1 minus k_{rl}. However, the important parameter for propagation of the pneumatic signal through the mountain is diffusivity, which is the ratio of the permeability to porosity of a model layer. The primary pathway for gas is assumed to be through the fractures in the densely welded formations, with matrix porosity adjacent to fractures also contributing to gas flow and signal attenuation because the gas is stored in the relatively large pore spaces. Thus, previous calibration efforts (Ahlers et al. 1996; Rousseau et al. 1998) have used a composite air-filled porosity estimate, smaller than the total matrix porosity but larger than the estimated fracture porosity, to calculate permeability from the diffusivity.

In this combined moisture and gas-flow model, the matrix porosity, as measured from core samples is used in the simulation of moisture flow during transient runs. The 1- k_{rl} formulation provides a high relative permeability of gas. This, coupled with the relatively large unsaturated matrix porosity available for gas storage in the DKM with one matrix grid block per layer, requires that the estimated fracture permeability in the model increase by several orders of magnitude in order to propagate the pneumatic signal down to the lower model layers. The increases were not consistent with the air-k test results reported by LeCain (1997, pp. 28-32). Therefore, the Brooks-Corey gas-phase relative-permeability model (Luckner et al. 1989, pp. 2187-2193) was instituted for the matrix to reduce krg, requiring smaller increases in fracture permeability during model calibration for the pneumatic data.

The matches to the pneumatic sensor data with the parameter set inversion, using the initial fracture m value of 0.492, are shown in Figures 6.4.3-1 and 6.4.3-2 of Bodvarsson et al. (1997, p. 6.45) for Boreholes SD-12 and SD-7, respectively. The plots show relatively good matches to the measurements from the sensors located in the upper layers of the model. The plot for SD-7 shows the lag between the signal as measured in the Tpp and Tptpmn (model layers PTn24 and tsw34, respectively). The model slightly underpredicts the signal amplitude observed in the lower sensors in the mountain. The resultant fracture-permeability parameter set obtained from the inversion is used as the base-case vertical fracture-permeability set.

The results show that the permeabilities of the fractures for the TCw and TSw increase during the inversion. The largest increase is seen in block tcwF1 adjacent to the top boundary. Some of the permeabilities increase by more than the standard deviations obtained from the air-k test results from LeCain (1997, pp. 28-32). This suggests that the effect of having the total matrix porosity available for gas storage still has a significant effect, even though the relative permeability in the matrix has been reduced through the use of the Brooks-Corey curve. The diffusivities calculated from the permeability and porosity data for the TSw layers are consistent with the results obtained through the FY-96 calibration of the gas model described in Ahlers et al. (1996).

The differences in permeabilities between the calibrated model and the LeCain data may also be related to the difference in the scale and time constant of the measurements, since the air-k tests measure relatively short intervals over small time scales, while the propagation of the gas signal throughout the mountain is related to mountain-scale effects at longer time scales. On average, the estimated permeabilities for the 0.492-parameter set using the constant reduction factor are smaller than those estimated using the upstream S reduction factor. This is because the matrix permeabilities estimated by the program for the constant factor set are generally smaller, so that the fractures become a preferred pathway for the gas flow. This is not true for layer tsw31, however, because the fracture block for the PTn25 layer above it has been changed to have matrix properties with significant storage. Therefore, the permeability in the tsw31 fracture block must be increased to propagate the gas signal to the lower layers without attenuation.

Effects of Perched Water Calibration

Four out of the five boreholes represented by one-dimensional columns in the layer-average calibration submodel have perched water. However, in one-dimensional column inversions, infiltration at the top boundary is assumed to move vertically through the column. Therefore, potential lateral diversion of flow as a result of relatively impermeable geologic formations leading to perching cannot be simulated by the submodel. High saturations and associated water potentials have been matched by the inversion program in the locations of perched-water layers (Bodvarsson and Bandurraga 1996; Bodvarsson et al. 1997 (Chapter 6), but the calibrated parameters for the layers in and under the perching locations are probably associated with fluxes that are overestimated because of diversion. The perching location is reported by Wu et al. (1998, pp. 37-40) to be the basal vitrophyre of the TSw model layer tsw37 for boreholes SD-9 and UZ-14, and possibly SD-12. The property calibration for the layers beneath the tsw37 for these boreholes may be affected by the perching. In Borehole SD-7, and possibly in SD-12, the zeolitic layer in the Calico Hills formation (model layer ch3zc) causes perching.

The inconsistency in the conceptual model used to perform the one-dimensional inversions is addressed in a sensitivity study in Bodvarsson et al. (1997; Chapter 6). It is also addressed by altering the calibrated one-dimensional inversion property sets in the full three-dimensional model to match saturation and water potential profiles and produce perched water and associated lateral diversion at the observed locations (Section 2.4.3.4). The base-case one-dimensional inversions have not attempted to match low saturation valleys in the observed data below the perched water bodies, because the vertical flow rates in the columns are probably overestimated because there is a lack of lateral diversion. Instead, the inversions match the averages of the data reported for each geologic formation represented by a model layer. There is also the possibility of using LBNL's parallel processing capability to perform full three-dimensional model inversions for future calibration work, which would incorporate lateral diversion effects in the inversion. The use of a full three-dimensional inversion model would increase defensibility in the current calibration process.

2.4.3.1.4 Base-Case Hydrologic Properties Used in TSPA-VA

Using the above calibration approach, LBNL developed what they believed to be the most reasonable estimate (as of 7/31/97) of parameters to be used with the UZ model for both liquid and gas flow. It was a combination of the "base" (Table 6.4.1-2 from Bodvarsson et al. 1997) and "fracture" (Table 6.4.3-1 from Bodvarsson et al. 1997) parameter sets and was named the "preliminary base case." Vertical fracture permeability for layers tcw11 down to tsw35 and horizontal fracture permeability for layers PTn21 down to PTn25 were from calibration with the in situ pneumatic pressure data. Horizontal fracture permeability for layers tcw11, tcw12, tcw13, and tsw31 down to tsw35 were set to the initial guess for fracture permeability, which were from air permeability tests performed in vertical boreholes and, as such, represented the best estimate of horizontal fracture permeability. All other parameters were from the "base" calibration to saturation and water potential data only.

Fracture porosity was taken from Table 7.15 of Bodvarsson et al. (1997). 2-D porosity values were used down through tsw34. Below tsw34 only 1-D porosity values were available, so 1-D values were used for layers tsw35 and below. The fracture porosity shown for PTn25 is the fracture porosity from Table 7.15 of Bodvarsson et al. (1997) times the matrix porosity. This value is given so that the diffusivity of layer PTn25 is correct. Fracture frequency was used for generation of the dual permeability mesh and is from Table 7.12 of Bodvarsson et al. (1997).

In light of recent information from simulations of the single-heater test (SHT) in the ESF, additional constraints were placed on the van Genuchten fracture air-entry (alpha) parameter, which indicates the size of the fracture aperture, used in the preliminary base case. Previous estimations of this parameter via calibration methods yielded apertures that were unrealistically small and fracture capillary pressure that were unrealistically high. In TH simulations of the SHTs, use of these small fracture alpha parameters yielded poor matches with observed data. As a result, a prescribed set of fracture alpha parameters (min, mean, and max) was derived (see Section 2.4.3.2.2) for each stratigraphic unit and used in the final base-case TSPA-VA parameter sets.

Finally, the base-case parameter sets used fracture-matrix multipliers that were calibrated to global classifications of welded, nonwelded, and zeolitic stratigraphic units. Together with the variations in present-day infiltration (Section 2.4.2.7) and ranges in fracture alpha parameters, the base case consisted of five calibrated parameter sets:

- Base infiltration ÷ 3 and the van Genuchten air-entry parameter at a minimum for each layer (see Table 2-19)

- Base infiltration ÷ 3 and the van Genuchten air-entry parameter at a maximum for each layer (see Table 2-20)

- Base infiltration and the van Genuchten air-entry parameter at the nominal "best estimate" for each layer (see Table 2-21)

- Base infiltration × 3 and the van Genuchten air-entry parameter at a minimum for each layer (see Table 2-22)

- Base infiltration × 3 and the van Genuchten air-entry parameter at a maximum for each layer (see Table 2-23).

The fault parameters for matrix and fractures, as described in previous sections, are given in Table 2-24, respectively. Nomenclature for the perched water zones and fault zones are given in Table 2-25 and Table 2-26, respectively.

Recommendations for Development of Future Parameters

Based on the results of the inversions presented above, LBNL recommends that the project pursue three-dimensional inversions using available parallel-processing capabilities to minimize the number of assumptions in the inversions (such as the use of one-dimensional submodels that do not capture the perched-water effects). The project also recommends that the three-dimensional inversions add data, such as temperature and geochemical measurements, to explicitly constrain infiltration rates, fracture/matrix equilibrium, and travel times during the three-dimensional inversions. These three-dimensional inversions would increase the defensibility of the current calibration process. Also, the creation of a heterogeneous property set should take advantage of the considerable data concerning parameter uncertainties developed in the one-dimensional models and with the heterogeneous distributions provided by Rautman and McKenna (1997, pp. 1-29) to generate a stochastic representation of the parameter fields in the site-scale UZ model.

2.4.3.2 Sensitivity Studies for Determining Important Hydrologic Properties

A series of UZ simulations has been performed to examine the sensitivity of water flow to matrix and fracture permeabilities and van Genuchten properties in a one-dimensional, dual-permeability system. These studies, in part, formed the basis for the choice of parameters that were used in the base case, as described in the previous section. These simulations are divided into two sets. In the first set presented, ranges in property values were defined using the properties and mean and standard-deviation values determined from inverse modeling done at LBNL (Bodvarsson et al. 1997, Chapter 7). Results from these simulations show that, for the ranges of values considered, the fraction of infiltrating water that travels downward through the fracture continuum is primarily controlled by fracture alpha and to a lesser extent fracture permeability. In this first set of simulations, the range of fracture alpha values considered was quite large relative to other property ranges and as a result its impact on flow behavior was most significant. To reduce the uncertainty in fracture-alpha values, a subsequent study by Altman (1997, Chapter 4) was conducted to derive more reasonable ranges of fracture alpha values. This study relied on published fracture-permeability and fracture frequency data and is presented following the first set of sensitivity studies.

A second set of simulations based on the new fracture-alpha ranges are then presented. In this set of simulations only two properties, fracture alpha and fracture permeability, were varied over their ranges. There were two important differences between this set and the first set of simulations: (1) a Weeps formulation was used; that is, the matrix-fracture conductance area was reduced by the fracture relative permeability to water; and (2) in addition to using the new fracture-alpha values, different minimum and maximum values of fracture permeability that are consistent with the new fracture-alpha values were also used. Results of this study show that, for the ranges of fracture permeability and fracture-alpha values considered, the fraction of infiltrating water that travels downward in the fracture continuum is controlled primarily by fracture permeability. To provide further insight into the relative importance of matrix and fracture properties, a dimensional analysis of the governing unsaturated-flow equations was also performed. This analysis is presented in the Section 2.4.3.2.4. Results of the dimensional analysis show that, in addition to relative permeability functions for the matrix and fracture continua, three dimensionless groups involving fracture and matrix properties characterize the properties of the UZ dual-permeability system.

2.4.3.2.1 Evaluation of Varying Permeabilities and van Genuchten Parameters on UZ Flow

A series of one-dimensional numerical simulations has been performed to evaluate the sensitivity of water flow to matrix and fracture properties. Permeability and van Genuchten parameters for both the matrix and fracture continua were varied in the simulations. Ranges in property values were defined using the base-case property set and mean and standard-deviation values determined from inverse modeling done at LBNL. Numerical simulations were run using TOUGH2 (SNL v3.4.1). This version allows for a modification of the connection area term between fractures and matrix. Simulations were run to 1 million years. The dual-permeability model (DKM) was used, allowing for flow through both matrix and fracture domains and between the two domains. All simulations and source data have been submitted to the Technical Data Base (SNT05091597001.004).

Description of Simulations

Simulations were run on a one-dimensional column at Nevada State Plane location N234,054 m, E171,280 m. This location corresponds to borehole SD-9. The grid used in the TOUGH2 simulations is shown in Figure 2-21. The cross-sectional area of each grid block is 6,810 m^2. The domain was divided into 22 elements. Each element represents one hydrostratigraphic unit, with the exception of the TSw5, which was split into three elements, and TSw6, which was split into two elements. These layers were split into more than one element in order to further refine the grid at the approximate elevations of the repository. One modification has been made to the layering used by LBNL. In the model the upper layer of the CHn is modeled by LBNL as a zeolitic layer. The reasoning behind this classification is that the layer is partially altered and that only the upper 4 m of the layer can be considered unaltered. Our reasoning for changing the layer to a vitric layer is that the low saturations at that elevation indicate that there is a vitric layer there.

The upper boundary has a constant infiltration rate of 3.6 mm/yr (7.76×10^{-4} kg/s). The water is introduced into the fracture domain. This infiltration rate is what is used on the LBNL site-scale model at the location of SD-9. The lower boundary of the model is set to water-table conditions. A natural thermal gradient is modeled on the column with a temperature of 19°C at the ground surface (Sass et al. 1988, pp. 8-49) and 32°C at the water table (Fridrich et al. 1994, pp. 133-168).

Hydrologic Properties

Fracture and matrix properties used in these simulations are parameters distributed by LBNL on April 29, 1997 (Note that these are different from the base-case property sets given in Table 2-19 through Table 2-24). The mean properties, along with the standard deviations for each property, were output by ITOUGH2. It should be noted that the standard deviations that were calculated by ITOUGH2 were strongly dependent on the initial guess of the standard deviation as input by the user. For the matrix parameters these standard deviations were based on the core-plug measurements (Flint 1998, pp. 44-45). The initial estimation for the fracture alpha and lambda standard deviations were more arbitrary.

"Minimum" and "maximum" parameter values were calculated as the mean minus or plus one standard deviation, respectively. The ranges of parameters are shown graphically in Figure 2-25 through Figure 2-27. This range of plus or minus one standard deviation accounts for 68.3% of the range of values. Thus, these analyses do not evaluate the 31.7% of the ranges of the parameters in the tails of the distributions (assuming a Gaussian model).

The range of measured matrix permeabilities as reported in Flint (1998, p. 44) is also presented in Figure 2-25. Note that in many of the TSw layers (Tsw1, Tsw2, Tsw4, and Tsw6) the maximum matrix permeability was larger than the mean measured permeability plus one standard deviation, as defined by the core-plug data. This is also true for some of the mean calibrated values of matrix permeability (TSw1 and TSw6).

There are other aspects of the matrix-permeability data of which the reader should be aware. The detection limit of the equipment on which the measurements were made was approximately 5×10^{-19} m^2. For many of the geologic layers a large portion of the samples yielded nondetectable permeabilities and were not used in determining the mean permeabilities for each layer. This leads to an overestimate of the matrix permeability values. For example, in the TSw middle nonlithophysal (TSw4), 28 out of the 39 samples measured had nondetectable permeabilities. If these samples are counted in the mean as being at the detection limit (again an overestimate) the mean permeability changes from 4.07×10^{-18} m^2 to 9.17×10^{-19} m^2. The upper TSw layer, the vitric caprock, has four out of seven samples at the nondetectable level. Accounting for these samples changes the mean permeability value from 7.78×10^{-17} m^2 to 4.40×10^{-18} m^2. These values are presented in Bodvarsson et al. (1997, Chapter 6).

An infiltration rate of 3.6 mm/yr in a saturated matrix translates to a saturated permeability of 1.2×10^{-17} m^2. This means that the matrix in almost every unit is capable of sustaining flow through it without getting saturated. The following layers are the exceptions: TCw1, TCw2, and the minimum values for TCw3, TSw4, TSw6, TSw7, CH3z, and CH4z.

Simulations were run using the minimum or maximum value for one parameter at a time. With three separate parameters for both the fractures and matrix (six parameters total), there are 12 simulations and one base-case simulation using the mean values for all of the parameters. All layers were changed to this minimum or maximum value. The one exception to this rule was for simulations using the minimum matrix permeability. Using the straight minimum values, the simulation could not reach steady state in a reasonable amount of time. To fix this problem the values used for the CH1v layer and CH3z layers were the mean minus one-half of the standard deviation.

The connection-area reduction term varies from unit to unit. To maintain consistency with the methods used by LBNL in doing the inversions, the upstream relative permeability was used as the multiplication factor to the geometric connection area for the welded units (TCw and TSw). The upstream saturation was used as the multiplication factor to the geometric connection area for the nonwelded units (PTn, CHn).

It should be noted that the input parameter in TOUGH2 (and ITOUGH2) is lambda (λ or m) instead of the more widely referred-to beta (β or n), where

$$\lambda = \left(1 - \frac{1}{\beta}\right) \text{ or } \beta = \frac{1}{(1-\lambda)} \tag{2-4}$$

The presentation and discussion of results below will refer to lambda instead of beta since that is the parameter that was used in the inversions, therefore, the parameter that was varied. It should be noted that, for the ranges in lambda values that were used here, an increase in lambda also means an increase in beta. A larger lambda or beta indicates a narrower pore-size distribution.

Fracture lambda, λ_f, was found to be an insensitive parameter when conducting the inverse modeling. Therefore, the calculated λ_f values will be close to what was given for the initial guess. In this case the initial guess was set to 0.492 (β_f=1.97). This value assumes a log-normal fracture aperture distribution with a standard deviation of 0.5. This aperture distribution is the higher end of the expected range. The lognormal standard deviation estimated from the air-permeability data is approximately 0.32. This standard deviation would imply a λ_f=0.63 (β_f=2.70) (Bodvarsson et al. 1997 (Chapter 6).

The fracture residual saturations were assumed to be 0.01, consistent with values discussed in Section 2.4.3.1.3. In examining the results of the simulations it can be seen that the fracture saturations do not approach this residual saturation value so as to affect the pore-water velocities.

Simulation Results

In examining the results of the simulations, three parameters were examined for both the fractures and matrix: saturations, normalized mass-flow rates (mass-flow rate/infiltration), and pore-water velocities. Matrix saturations are important to examine to make sure that the values are still within the range of the measured core-plug data. It is expected that there will not be much of a discrepancy between the measured and simulated matrix-saturation data since those data were used in the inversion process. The fracture saturations are important in that they are inversely related to the fracture pore-water velocities, an important parameter for transport. Mass flow rates are important to make sure the simulations are consistent with the conceptual model used in the inversion process. Mass-flow rates are also directly related to pore-water velocities. Finally, pore-water velocities are likely the most important parameter to TSPA. This is the parameter that is the indication of the travel times of radionuclides through the UZ. For this reason, the discussion of the velocities concentrates on the repository horizon and below. It should be noted that, for the simulations run in the area below the repository, the fracture pore-water velocities were orders of magnitude larger than the matrix pore-water velocities.

Matrix Permeability

Results to changes in km are presented in Figure 2-28. Fracture saturation in the CHn changed by approximately 10% by varying the matrix permeability. The variation was not enough to counterbalance the changes in mass-flow rates (approximately 15% in the CHn and 25–30% in the lower TSw). Therefore, an increase in matrix permeability leads to a decrease in fracture pore-water velocities. The range in pore-water velocities over the range in matrix permeabilities was a little more than an order of magnitude in the CHn. The effect on the fracture pore-water velocities in the TSw were minimal.

Fracture Permeability

Results of varying k_f are presented in Figure 2-29. Changes in k_f had only minor effects on both S_m and S_f. The largest changes (approximately 10%) were in S_m in the TSw from the lower lithophysal layer and the layers above. These ranges are well within the variation of the core-plug data. Mass-flow rates varied as expected. Decreasing the k_f leads to almost 100% of the flow in the matrix in the CHn. Increasing the k_f leads to an increase from when the mean k_f is used in fracture mass-flow rates in the CHn by 20–25%. In the TSw the mass-flow rates ranged over 20% with changes in k_f.

Changes in fracture pore-water velocities are therefore expected to be controlled by the changes in the fracture permeability, k_f. Fracture pore-water velocities ranged over almost two orders of magnitude in the CHn with the variations in k_f. Changes in fracture pore-water velocities in the TSw were much less, varying by approximately a factor of two.

Matrix Alpha

Results of varying matrix alpha are presented in Figure 2-30. Mass flow rates changed only minimally. Normalized mass-flow rates ranged only over less than 10% in the CHn and 10–15% in the lower TSw. Therefore, as would be expected with these small changes in saturations and mass flow rates, the fracture pore-water velocities did not vary to much over the range of changing am. The maximum change appears to be by approximately a factor of three in the CHn.

Fracture Alpha

Results of varying fracture alpha are presented in Figure 2-31. The saturations ranged over a larger area than is observed by varying the other parameters. Fracture saturations ranged over approximately 15% in the CHn and as much as approximately 25% in the TSw basal vitrophyre. Matrix saturations varied by as much as approximately 25% in the TSw lower lithophysal and 40% in the TSw rounded unit. Fracture pore-water velocities in the CHn ranged over almost two orders of magnitude. In the lower TSw the range was approximately one order of magnitude. It is interesting to note that, in the two lower units in the TSw, the fracture pore-water velocity using the mean α_f actually exceeds the pore-water velocity when the minimum α_f values are used. When the minimum α_f is used in the simulations, the mass flow in the TSw is almost all in the fractures do not vary much throughout the unit. Fracture pore-water velocities are very close to each other in the middle portions of the TSw, whether the mean or minimum α_f is used in the simulations. You will notice that the fracture saturations increase in the lower two units. This increase is enough without any relative changes in mass flow rates, so that pore-water velocity in the lower two units of the TSw decrease to slower velocities than were simulated using the mean α_f values.

Examination of the results of the simulations show that increasing the α_f within the ranges given by ITOUGH2 can lead to fracture mass flow rates so low in the TSw that the mass flow rate of the matrix exceeds the mass flow rate of the fracture (Figure 2-31). This result does not match our conceptual model of flow being fracture dominated in the welded units. In this case, increasing the α_f has decreased the suction pressure of the fractures in the TSw enough so that most of the water stays in the matrix.

These results also call attention to the k_m values being used in this column. The values presently being used are high enough to sustain the majority of flow in the welded units through the matrix. In the TSw, it is only at the TSw4 that the matrix is almost saturated when the maximum α_f values are used in the simulations. As discussed in the parameters section, the k_m being used are overestimates because the nondetect measurements are not used in calculating mean values.

To better bound α_f values, simulations were run where the α_f was changed by adding or subtracting only one-half of the standard deviation. Remember that the standard deviations given as output in the ITOUGH2 simulations are very dependent on what the initial estimate is set at. In this case, the initial estimate was set so the α_f could vary by an order of magnitude [log(standard deviation)=1], a somewhat arbitrary number.

Changing the α_f values by one-half an order of magnitude allowed more water to stay in the fractures in the TSw, but the matrix mass-flow rates still exceeded the fracture mass-flow rates (Figure 2-32). In this case a little more than 40% of the water flowed through the fractures while a little less than 60% flowed through the matrix. For values of α_f less than the mean value, the fracture pore-water velocities in the CHn range over approximately one order of magnitude (as opposed to the two orders of magnitude when the full range of α_f is used) (Figure 2-32). For values of α_f less than the maximum values, the ranges of pore-water velocities in the TSw are approximately a factor of two or three.

Matrix Lambda

Results of varying matrix lambda are presented in Figure 2-33. Fracture pore-water velocities do not appear to be affected by increasing λ_m, and the pore-water velocities in the lower CHn increase by a factor of two to three by decreasing the λ_m.

Fracture Lambda

Figure 2-34 presents the results of the simulations with a variation in the λ_f for all of the layers. Changing λ_f has more of an effect on the system than changing λ_m. Fracture saturations ranged over a span of approximately 15%. Fracture mass-flow rates in the TSw range over 20–25%. Mass-flow rates in the CHn did not vary as much. The counterbalancing effects of an increase in fracture mass-flow rates and a decrease S_f in lead to a smaller range of fracture pore velocities: approximately a factor of two in the CHn and TSw.

Discussion of Simulation Results

Fracture pore-water velocity is an important output parameter to examine to determine the sensitivity of the input parameters for TSPA. This is because the pore-water velocity will significantly affect transport of radionuclides in the UZ. In examining the fracture pore-water velocities for the simulations discussed above, it can be concluded that, for the range of property values considered, fracture alpha and fracture permeability are the two most important parameters.

In evaluating the simulation results, it is important to account for their dependency on the conceptualizations of fracture-matrix interactions. In this case the fracture-matrix conductance term is much higher in the nonwelded units than in the welded units. Using a model with a reduction term of the upstream relative permeability for all units or the upstream saturation for all units could lead to different results. To test this hypothesis, several simulations were performed using different conceptual models of fracture-matrix interactions (see Section 2.4.3.3).

These simulations indicate that using different conceptual models for the TSPA-VA calculations might be more important than varying certain parameters. It was shown that the ranges of pore-water velocities over the ranges of λ_f did not change significantly for the different conceptual models. Ranges in pore-water velocities over the ranges of k_f decreased from approximately two orders of magnitude for the base case to less than an order of magnitude for the two alternative conceptual models for fracture-matrix interactions. Also, the differences in the matrix permeabilities for the CH1z unit between the different parameter sets for the different conceptual models was greater than the variability within one parameter set.

As a final note, there is one parameter that was not examined in this suite of simulations that is important to radionuclide transport calculations. Fracture porosity is a parameter for which there is significant uncertainty (over an order of magnitude). Fracture porosity was not calculated by the inverse model nor varied in these sensitivity studies, because it is not included in the governing equations for steady-state flow simulations. However, fracture porosity has a strong effect on pore-water velocities (calculated by dividing the percolation flux by the product of the liquid saturation and porosity) and is therefore important to radionuclide transport, which is considered in Chapter 7 of the Technical Basis Documents.

2.4.3.2.2 Determination of Reasonable Ranges for van Genuchten Fracture Alpha

In the foregoing sensitivity analyses, performance measures of pore-water velocity and mass-flow rates for the base-case parameter set were found to be strongly sensitive to fracture alpha. In this section, suggested ranges in van Genuchten fracture alpha (α_f) are developed. The analyses presented here are a continuation of the work reported in Bodvarsson et al. (1997, Chapter 7). This section summarizes the methods for calculating α_f from the available data and reports mean values of α_f (DTN: SNT05091597001.003).

The equation used to calculate α_f [m^{-1}] is as follows:

$$\alpha_f = \frac{b \rho g}{2 \tau \cos\theta} \qquad (2\text{-}5)$$

where b is the fracture aperture (m), ρ is the density of water at 20°C (998. kg/m^3), g is the acceleration due to gravity (9.80 m/s^2), τ is the surface tension of water at 20°C (0.072 N/m), and θ is the contact angle (equal to zero if water is assumed to completely wet the fracture surface). Equation (2-5) is derived from the Young-Laplace equation assuming a plane fracture. It can be seen from Equation (2-5) that fracture aperture is an unknown. Unfortunately, there are no direct measurements of fracture aperture, so it also needs to be calculated. The equation used to calculate aperture is as follows:

$$b = \sqrt[3]{\frac{12 k_f}{F_f}} \qquad (2\text{-}6)$$

where k_f is the fracture permeability [m^2] and F_f is the fracture frequency [m^{-1}]. Equation (2-7) is derived from the cubic law for fracture permeability (Domenico and Schwartz 1990, pp. 86-87), which assumes steady, fully developed, laminar flow in a plane fracture (Poiseuille flow). The above two equations, along with published measurements for k_f and F_f, are used to determine reasonable ranges for fracture alpha.

Available Fracture Data

Fracture permeability data were taken directly from Table 7.12 of Bodvarsson et al. (1997, Chapter 7) and Table 6.4.3-1 from Bodvarsson et al. (1997, Chapter 6). Both tables report mean log10 k_f and standard deviations of the log10 k_f distributions. Table 7.12 summarizes the results of air-permeability measurements made in the boreholes. The DTN for source air permeability data is GS960908312232.013 (LeCain 1997). Table 6.4.3-1 of Bodvarsson et al. (1997, Chapter 6) summarizes the results of inverse modeling using the in situ barometric-pressure measurements. It can be observed that the air-permeability measurements yield higher permeability values than those calculated from the inversions for the Paintbrush Tuff nonwelded unit (PTn) units. Based on this observation it was thought that the air permeability measurements might have been measuring some matrix permeability in the PTn. Therefore, it was decided to use the permeability values from Bodvarsson et al. Table 6.4.3-1 for PTn layers. This is consistent with what was used for the base-case parameter set. It should also be noted that standard deviations for the air-permeability measurements were not available for some layers. The DTN for the data presented in both Bodvarsson et al. (1997, Chapter 7) and Bodvarsson et al. (1997, Chapter 6) is LB970601233129.001.

There are two sources of fracture frequency (F_f) data: measurements taken in the ESF and those taken from borehole core. The ESF data used to calculate the fracture spacing was from the DLS. The DTNs for these data are presented in Table 2-27. Data from the ESF go only to the middle of the Topopah Spring welded unit (TSw) (TSw34 in the UZ model layer nomenclature). Therefore, borehole data were used for F_f values in the deeper layers. The F_f borehole data come from two separate boreholes: SD-12 (DTN: SNF29041993002.071 (Rautman and Engstrom, 1996, pp. 22-26)) and NRG-7a (DTNs: SNF29041993002.015 and SNF29041993002.048).

Bodvarsson et al. (1997, Chapter 7) did an extensive job of evaluating the data and presented arithmetic mean values for F_f. In evaluating the ESF data, fractures less than 1 m long were discarded. The length of the fractures cannot be determined from borehole core, so Bodvarsson et al. (1997, Chapter 7) presented a method of "correcting" the fracture data.

Methodology for Determining Ranges in Existing Fracture Data

Fracture Permeability

As the means and standard deviations were available for the k_f data, determining bounds was relatively straightforward. In this study, a range of two standard deviations on either side of the mean was used, which, assuming that the $\log 10 k_f$ are normally distributed, encompasses approximately 95% of the values. The following equations were used to calculate the extreme values.

$$k_{f\,\min} = 10^{((\overline{\log(k_f)}) - 2SD)}; \qquad k_{f\,\max} = 10^{((\overline{\log(k_f)}) + 2SD)} \tag{2-7}$$

The k_f data are presented in Table 2-28. The mean $\log k_f$ values from Equation (2-7) are in column 1 and the standard deviations (SD) are in the second column. Note that, for five layers, standard deviations were not available. For these layers, only mean values were used and the variation in the α_f was determined solely from the F_f data.

Fracture Frequency or Fracture Spacing

Determining ranges of F_f is not as straightforward because of different sources and forms of the data. From the ESF DLS data, fracture spacings can be calculated directly. The minimum measurement precision in the measurements was 0.01m. Because of this minimum, it was possible to obtain fractures that had zero spacing. Data of fracture spacing in the ESF indicate a lognormal distribution rather than a normal distribution (Tables 7.7 and 7.8 in Bodvarsson et al. 1997); therefore, with zero spacing values, it is not possible to determine the geometric mean of the distributions. Therefore, zero values were set to 0.005 m (one half the precision of the measurement). There were not enough of these values to have a large effect on the calculations, but it was thought that the data should not just be discarded. In plotting the data it can be seen that the distribution is not quite lognormal (Figure 2-35). Also, for some of the layers not enough data were available to define a good distribution. Based on these observations, it was decided to use the 10th and 90th percentile point in the distributions to define the range in fracture spacing. From these data F_f can be directly calculated as the inverse of fracture spacing. These values are presented in Table 2-29. It should be noted that it was decided to combine all the data for the PTn into only one distribution for the whole nonwelded layer. This decision was made based on three factors: (1) lack of data to adequately characterize most of the individual layers, (2) the location of the PTn well above the repository, and (3) lateral flow in the PTn is not considered an important factor for the overall potential repository performance (CRWMS M&O 1997).

Examination of Table 2-29 shows that the mean F_f's that were calculated are not identical to those presented in Bodvarsson et al. (1997, Chapter 7). Bodvarsson et al. (1997, Chapter 7) used an arithmetic mean as reported in Equation 1 of that report. Differences in values for the TCw layers can be explained by the fact that Bodvarsson et al. (1997, Chapter 7) calculated mean spacings for different subunits within the TCw layers and then averaged those values. In contrast, in this study all the sublayers were combined to calculate one spacing value for each layer. This means that the different sublayers take equal weighting despite possibly different thicknesses. One other difference in the calculation methods is that zero spacings were set to 0.005 while Bodvarsson et al. (1997, Chapter 7) kept them at zero. Nevertheless, the differences in the mean F_f are small and are not particularly germane to the objective at hand. For the purposes of determining ranges of fracture alpha for use in TSPA-VA, the geometric means of fracture frequency in Table 2-29 were used.

The ESF does not enter any layers below the TSw34. For these layers Bodvarsson et al. (1997, Chapter 7) resorted to borehole data. There are only two boreholes for which F_f data are available for these lower layers: NRG-7a and SD-12. The borehole data are reported as the number of fractures per 10-foot section of core. Bodvarsson et al. (1997, Chapter 7) took those data and corrected for percent recovery of the core and the dip of the fractures. With the ESF data, fractures shorter than 1 m were not included in the determination of F_f. However, the length of the fractures is unknown with the borehole data. For this reason Bodvarsson et al. (1997, Chapter 7) also calculated a correction factor to the borehole data to reduce the F_f to what would be expected if only the longer fractures were counted. Use of the correction factor produces only an approximation of the expected F_f.

Fracture-frequency data from the boreholes are presented in Table 2-30. Again, there are some differences between how Bodvarsson et al. (1997, Chapter 7) calculated the mean F_f and how the calculations presented here were performed. Namely, Bodvarsson et al. (1997, Chapter 7) determined a mean F_f for each borehole and took the mean of those two values. In the case of the Calico Hills zeolitic units, core from SD-12 intersected two different units (CH1zc and CH3zc). These units (along with that intersected in NRG-7a) were weighted equally. The mean values presented here combined all of the units (within and between boreholes) so that the F_f would be weighted by the thickness of the units in each borehole.

Examination of Table 2-30 shows some of the complications in using the borehole data. First, there are not that many samples, especially for the TSw37 and Calico Hills layers. Second, for almost every layer there are 10-foot sections of core in which there were no fractures. Including these data in defining the distributions is not straightforward. Finally, in comparing the layers TSw32 - TSw34 (where both sets of data exist) it can be seen that the maximum fracture frequency for the borehole data is much less than that for the ESF data.

Given all of these complications, it was decided to use analog layers for these lower layers instead of using the borehole data. The analogs and their reasoning are presented in Table 2-31. While some of the reasonings for picking the analog layers have weaknesses, comparing Table 2-29 and Table 2-30 shows that, in all the cases, using the analogs increases the range of fracture frequencies. Therefore, by using the analogs instead of the borehole data, the variability in the parameters was increased. Using the analogs also helps define the lower end of the distribution, something difficult to define with the borehole data.

Both the CHz and PTn are nonwelded. The PTn most likely has a wider range of F_f than CHz. Using this wider range for the CHz F_f increases the uncertainty in CHz F_f. Increasing the uncertainty seems to be the best option without a better alternative for bounding the CHz F_f.

Discussion of Results

With the ranges of k_f and F_f defined, it is possible to define the α_f ranges using Equation (2-6) and Equation (2-7). The final information used to calculate the α_f distribution is summarized in Table 2-32. The final distributions of α_f are summarized in Table 2-33.

In order to evaluate the α_f distributions, a more statistically rigorous analysis was used to define an α_f distribution. This method was used on only one layer (TSw33) in order to make comparisons. For this example both the air-permeability and ESF fracture-spacing data were fit with log-beta distributions (see Harr 1987, pp. 79-91) for an explanation of the beta function). The air permeability distribution was cut off at four standard deviations on either side of the mean. The fracture spacing distribution was cut off at the minimum and maximum of the data. A fracture spacing of 0 m was set to 0.005 m. The mean and standard deviation for the k data were those reported in Table 7.12 of Bodvarsson et al. (1997, Chapter 7). For the fracture-spacing data, the mean and standard deviations were calculated from the data. The important parameters for the distributions are summarized in Table 2-34. The variables, p and q in Table 2-34 refer to fitting parameters for the log-beta distributions.

With these two distributions, parameters were sampled randomly 100 times, and these parameters were used to calculate an α_f distribution using Equation (2-5) and a modification of Equation (2-6). Equation (2-6) was modified into Equation (2-8) as fracture spacing was used instead of F_f (a_f=1/F_f).

$$b=\sqrt[3]{12k_f a_f} \tag{2-8}$$

The final distribution for TSw33 is presented in Figure 2-36. Annotating this distribution are the values recommended for use in TSPA-VA, along with other α_f values that were offered in the preliminary base case or other publications. It can be seen that the suggested bounds yield fairly extreme values in the distribution. However, the range of the distribution is still only approximately 1.5 orders of magnitude, showing that there is not a lot of variation in α_f if our calculation methods are valid. It is also interesting to note that the α_f, used for this layer in the preliminary base-case parameter set (7/31/97) falls completely outside the calculated range that is presented. The extremely small values of α_f in the preliminary base case prompted the effort to determine more reasonable values for this parameter in the final base case used in TSPA-VA.

There are several more layers in the LBNL site-scale UZ flow model that have not been listed in the tables in this section. As with the base-case parameter set, analog layers are used. It is proposed to use the same analogs for the α_f data. All the zeolitic units (ch1zc, ch2zc, ch3zc, ch4zc, pp2zp, and bf2zb) should take on the values of CHz presented in Table 2-33. The vitric layers (ch1vc, ch2vc, ch3zc, ch4zc, pp3vp, bf3vb, and tm3vt) should take on the values reported as CHv in Table 2-33.

Finally, it should be noted that in layers CHz and PTn, mean fracture-alpha values reported in Table 7.13 of Bodvarsson et al. (1997, Chapter 7) fall outside the range of fracture-alpha values given in Table 2-33. The reason for the discrepancies lies in the different methods used for determining fracture frequency, F_f.

In the case of the PTn, it was decided that there were not enough data to treat each layer of the PTn individually and that it was more appropriate to use a single range of F_f for the whole PTn. The range used in this study was 0.23–4.35 1/m. For the PTn22 and PTn23 layers, Bodvarsson et al. (1997, Chapter 7) calculated F_f of 0.29 1/m. This value was based on measurements for three fractures in the PTn22 and six in the PTn23. These layers have the fewest data points. The lumped PTn range determined in this study is based on 100 data points. The other difference in methods is that this study used the pneumatic-inversion permeabilities instead of air-k that Bodvarsson et al. (1997, Chapter 7) used. It was thought that the air-k measurements in the PTn might have been measuring some matrix k also, thus explaining why air-k measurements are higher than what was calculated by the inversion method. In the case of the PTn23 layer the differences in permeabilities were approximately an order of magnitude. Therefore, these differences in F_f and fracture-permeability measurements were sufficient to make mean fracture alphas in Bodvarsson et al. (1997, Chapter 7) fall outside the range of fracture alpha in the PTn23.

For the CHz, a different method than the one used by Bodvarsson et al. (1997, Chapter 7) was used in this study for calculating F_f. The F_f value in Bodvarsson et al. (1997, Chapter 7) is based on borehole data. Only two boreholes encountered the Chz. Bodvarsson et al. (1997, Chapter 7) took the mean F_f (fracture encountered per 10 feet) for each of the two boreholes and averaged them. In one of the boreholes, no fractures were resulting in a very low F_f for the CHz (0.067 1/m). In this study, the PTn was used as an analog for the CHz. This gave a range of F_f of 0.23–4.35 1/m, which is larger than what Bodvarsson et al. (1997, Chapter 7) calculated. The F_f in Bodvarsson et al. (1997, Chapter 7) falls well out of the range of F_f determined in this study, which is why mean fracture alpha also falls outside of the range in the CHz.

2.4.3.2.3 Evaluation of Varying Fracture Permeability and van Genuchten α_f on UZ Flow

A series of simulations was performed to examine the sensitivity of water flow to fracture permeability and van Genuchten fracture alpha in a one-dimensional, dual-permeability system. This dual-permeability system is modeled using a "Weeps" formulation that reduces the fracture-matrix conductance area by a factor equal to the fracture relative permeability to water (Ho 1997, pp. 407-410). In this sensitivity study, only two factors, α_f and k_f, were varied over their ranges. These two parameters were selected for analysis based on the results of the previous sensitivity study described in Section 2.4.2.2, which showed that α_f and k_f strongly influence how liquid flow is proportioned between the matrix and fracture continua.

In these simulations, mean values for α_f and k_f and all other parameter values are equal to values specified in the DKM/Weeps mean property set (DTN LB971100001254.004). The α_f and k_f values used in this study are given in Table 2-35. Note that the mean α_f values in Table 2-35 correspond to the DKM/Weeps mean property values for α_f and in some cases fall outside the range of the minimum and maximum values determined in Section 2.4.2.2.2 and presented in Table 2-33.

Simulation results show that, for the range of fracture permeability and fracture-alpha values considered in this study, the fraction of infiltrating water that travels downward through the fracture continuum is primarily controlled by fracture permeability.

Description of Simulations

Seven simulations were performed for the following combinations of α_f and k_f:

1. Mean values for both α_f and k_f
2. Mean α_f and maximum k_f
3. Mean α_f and minimum k_f
4. Maximum α_f and mean k_f
5. Minimum α_f and mean k_f
6. Minimum α_f and maximum k_f
7. Maximum α_f and minimum k_f.

The latter two simulations were selected because it was suspected that these parameter combinations would yield the maximum and minimum fracture-flow conditions; minimum α_f tends to promote the transfer of liquid to the fractures and maximum k_f increases the flow conductance of the fractures. The opposite conditions occur for maximum α_f and minimum k_f.

All simulations were performed using a vertical one-dimensional column representation of Yucca Mountain corresponding to a location at a northing coordinate of approximately 233,400 m and an easting coordinate of 170,650 m. The column was discretized using a finite-volume mesh comprising 51 pairs of matrix and fracture grid blocks. Each finite-volume element of the one-dimensional mesh is 15.81 m wide and 15.81 m thick, and the height of each element varies so that the discretization is finer near the repository. The matrix and fracture blocks include 5 pairs for the welded Tiva Canyon (TCw), 5 pairs for the nonwelded paintbrush (PTn), 21 pairs for the welded Topopah Springs (TSw), and 20 pairs for the Calico Hills (CH, PP, and BF3).

Water infiltration was introduced at the top fracture element of the model domain at a steady rate of 3.6 mm/yr. At the bottom of the column, an additional element was added to simulate a water table with prescribed pressure and saturation. All simulations were performed for a period long enough (1.0E06 years) for steady-state conditions to be achieved. All simulations were performed using TOUGH2 (SNL v.3.1.2).

Discussion of Simulation Results

A key metric for evaluating the sensitivity of water flow to α_f and k_f is the fraction of flowing water that travels through the fractures as opposed to the matrix continuum. This metric is important because the quantity of water flowing through the system potentially influences the quantity and concentration of contaminants leaving the repository. Moreover, it is important to estimate what fraction of flowing water travels through the fractures as opposed to the matrix continuum since contaminant travel times to the water table are typically significantly shorter when the main flow pathway is through fractures. Travel times are directly related to pore velocities and for this reason pore velocities are also an important metric.

Normalized mass flow rates (mass flow rate divided by infiltration (3.6 mm/yr)) and pore velocities for all seven simulations are shown in Figure 2-37 and Figure 2-38. Figure 2-37 and Figure 2-38 show that the proportion of mass that flows in the fracture continuum is primarily a function of fracture permeability. Very little change in mass flow is seen when fracture permeability is held constant and fracture-alpha is varied. Because the change in fracture alpha has little impact on flow, the combinations of minimum and maximum fracture permeability with minimum and maximum fracture alpha produce results very similar to the minimum and maximum fracture-permeability simulations. Similar conclusions can be drawn from the fracture and matrix pore-velocity results shown in Figure 2-39 and Figure 2-40. Finally, it was found that matrix and fracture saturations for the minimum and maximum fracture cases do deviate from the mean case; however, they fall within an acceptable range close to the DKM/Weeps mean property model. Representative saturation results are shown in Figure 2-41. Similar saturation results were obtained for the other simulation cases.

2.4.3.2.4 Dimensional Analysis of Governing Flow Equations

The main purpose of performing a dimensional analysis is to provide additional insight into the relative effects of matrix and fracture properties on water flow. In this section, the equations governing variably saturated, one-dimensional, vertical flow of liquid in dual-permeability media are nondimensionalized to obtain dimensionless groups that represent the relative effects of matrix and fracture properties on water flow. Dimensionless groups can be useful in the present context because they define relationships between parameters that must remain constant in order for dependent variables such as matrix saturation to be invariant for different choices of uncertain parameter values. Knowledge of such relationships is valuable because it can be used to help constrain values of parameters for which measurements do not exist so that, for example, predicted saturations stay within the bounds of known data ranges.

The equations governing variably saturated, one-dimensional, vertical flow of liquid in dual-permeability media can be written as (Peters and Klavetter 1988, pp. 416-430; Pruess 1991, pp. 10-26, and Ho 1997, pp. 401-410):

$$\frac{\partial}{\partial z}\left[\frac{\rho_l k_m k_{ml}}{\mu_l}\left(\frac{\partial P_{ml}}{\partial z}-\rho_l \bar{g}\right)\right]=\frac{\partial(\rho_l\,\phi_m\,S_{ml})}{\partial t}+\frac{\rho_l k_m k_{ml}}{\mu_l}\frac{\sigma}{d}X_{fm}k_{fl}\left(P_{ml}-P_{fl}\right)-Q_{ml} \quad (2\text{-}9)$$

$$\frac{\partial}{\partial z}\left[\frac{\rho_l k_f k_{fl}}{\mu_l}\left(\frac{\partial P_{fl}}{\partial z}-\rho_l \bar{g}\right)\right]=\frac{\partial(\rho_l\,\phi_f\,S_{fl})}{\partial t}-\frac{\rho_l k_m k_{ml}}{\mu_l}\frac{\sigma}{d}X_{fm}k_{fl}\left(P_{ml}-P_{fl}\right)-Q_{fl} \quad (2\text{-}10)$$

where Equation (2-9) describes the flow of liquid (subscript l) in the matrix continuum (subscript m) and Equation (2-10) describes the flow of liquid in the fracture continuum (subscript f), and

k_{jl} = relative permeability to the liquid phase

k_j = intrinsic permeability (m^2)

μ_l = dynamic viscosity of the liquid (Pa-s)

P_{jl} = liquid pressure (Pa-s)

Q_{jl} = external source of liquid mass, (+) injection and (-) extraction (Kg/m^3-s)

ϕ_m = porosity

ρ_l = density of the liquid (Kg/m^3)

σ = specific surface of the interface between the fracture and matrix continua (m^{-1})

d = is the characteristic half width of the matrix continuum between fractures (m)

X_{fm} = reduction factor for the interface area between the fracture and matrix continua

z = depth taken to be positive upward (m)

with j = m,f.

Note that in Equations (2-9) and (2-10), the fracture relative permeability to water is included in the matrix-fracture liquid transfer term (Ho 1997, p. 402). This additional term effectively reduces the interfacial area for liquid conductance between fracture and matrix continua and is the basis for the Weeps formulation of the (DKM/Weeps).

Liquid pressure in the matrix and fracture continua are related to air and capillary pressure by the following relationships

$$P_{jl} = P_{jg} - P_{jc} \tag{2-11}$$

where P_{jg} and P_{jc} denote air and capillary pressure in the j-th continuum (j=m,f). In this study, the van Genuchten capillary pressure and relative permeability relationships are given by (Pruess (1987, pp. 74-78)):

$$P_{jc} = \frac{1}{\alpha_j}[S_{je}^{-1/m_j} - 1]^{1-m_j} \tag{2-12}$$

$$k_{jl} = S_{je}^{1/2}(1-(1-S_{je}^{1/m_j})^{m_j})^2 \tag{2-13}$$

where m_j and α_j are fitting parameters for the j-th continuum. The effective liquid saturation is

$$S_{je} = \frac{S_{jl} - S_{jlr}}{1 - S_{jlr}} \tag{2-14}$$

where S_{jlr} represents the residual liquid-phase saturation in the j-th continuum.

In this study, it is assumed that movement of air is insignificant and that air pressure in the matrix and fracture continua is constant and equal to atmospheric pressure. Previous studies have shown that this "single-phase" approximation (Richards' equation) is appropriate for the problem of interest (Ho et al. 1995, Chapter 2, pp. 5-7). It is further assumed that: (1) liquid density and viscosity are constants, (2) k_m and α_m are constant within a hydrologic layer, and (3) steady-state conditions prevail. Invoking the aforementioned assumptions, multiplying Equations (2-9) and (2-10) by the ratio α_m/k_m, Equations (2-9) and (2-10) can be rewritten in the following nondimensional form

$$\frac{\partial}{\partial \bar{z}}\left[k_{ml}\left(\frac{\partial \bar{P}_{mc}}{\partial \bar{z}} + \frac{N_\alpha}{1+N_\alpha}\bar{\gamma}\right)\right] = -N_A k_{ml} k_{fl}\left(N_\alpha \bar{P}_{fc} - \bar{P}_{mc}\right) - \bar{Q}_{ml} \tag{2-15}$$

$$\frac{\partial}{\partial \bar{z}}\left[N_k k_{fl}\left(N_\alpha \frac{\partial \bar{P}_{mc}}{\partial \bar{z}} + \frac{N_\alpha}{1+N_\alpha}\bar{\gamma}\right)\right] = N_A k_{ml} k_{fl}\left(N_\alpha \bar{P}_{fc} - \bar{P}_{mc}\right) - \bar{Q}_{fl} \tag{2-16}$$

where

$$N_A = \frac{\sigma L^2 X_{fm}}{d} \tag{2-17}$$

$$N_\alpha = \frac{\alpha_m}{\alpha_f} \tag{2-18}$$

$$N_k = \frac{k_f}{k_m} \tag{2-19}$$

with

$$\bar{\gamma} = \rho_l \bar{g}\left(\alpha_f + \alpha_m\right)L \tag{2-20}$$

$$\bar{Q}_{jl} = \frac{\mu \alpha_m L^2}{\rho_l k_m} Q_{jl} \tag{2-21}$$

$$\overline{P}_{mc} = P_{mc}\alpha_m \tag{2-22}$$

$$\overline{P}_{fc} = P_{fc}\alpha_f \tag{2-23}$$

and

$$\overline{z} = z / L \tag{2-24}$$

where L is a characteristic length of the system.

Equations (2-15) through (2-24) show that, in addition to the relative permeability functions, three dimensionless groups characterize the properties of liquid flow in the one-dimensional system considered here: N_A is a measure of the effective interfacial area per unit volume of soil available for liquid transfer between the fracture and matrix continua (as this number increases the resistance to liquid transfer between the matrix and fracture continua decreases); N_α is a measure of the capillarity contrast between the matrix and fracture continua (as this number increases capillarity in the fracture relative to the matrix increases, causing the liquid to favor occupation in the fracture continuum;) and N_k is a measure of the intrinsic permeability contrast (as this number increases flow in the fractures is favored).

Note that the number of physical property parameters in the system has been reduced from nine parameters (i.e., k_{ml}, k_{fl}, k_m, k_f, σ, d, X_{fm}, α_m, and α_f) to 5 (k_{ml}, k_{fl}, N_A , N_α, and N_k). One approach to performing a general sensitivity analysis is to estimate a range of values for each dimensionless group based on property values of its constituent parameters. A sensitivity analysis can then be performed by varying the dimensionless numbers simultaneously over their ranges. The reduction in parameters is advantageous since the number of independent factors that needs to be varied is reduced.

Based on dimensionless group N_α, it appears that α_m and α_f are equally important in their influences on predicted system behavior. Similarly, it can be concluded that k_f and k_m are equally important based on dimensionless group N_k. However, the actual impact and importance of a parameter on system behavior is also determined by the distribution and range of input values assigned to a parameter.

2.4.3.3 Fracture-Matrix Interactions

Dual-permeability models have been used to explicitly model unsaturated-groundwater flow and heat through both fractures and matrix (Altman et al. 1996, pp. 15-17; Ho et al. 1995). In the DKM, the fractures and matrix are treated as separate discrete continua. Heat, gas, and liquid are allowed to flow between the fractures and matrix, as well as through each continuum. While the DKM is generally more applicable to a wider range of problems than the ECM (e.g., transient flows, high infiltration boundaries), the DKM requires additional information about the coupling between the fracture and matrix continua. Models have been proposed to accurately account for fracture-matrix interactions (Zimmerman et al. 1993, pp. 2127-2137; Gerke and van Genuchten 1993, pp. 1225-1228), but few of these have considered combined, unsaturated, heat and mass flow. Previous studies have demonstrated that the fracture-matrix coupling used for liquid flow in unsaturated DKMs may be significantly overestimated (Ho et al. 1995, Altman et al. 1996, pp. 15-17). Heterogeneities that cause flow channeling and fingering act to reduce the available area for liquid flow between the fracture and matrix continua. The purpose of this section is to present a model for unsaturated heat and mass flow between fracture and matrix elements in the DKM. Theory is presented to illustrate the need for modifications to geometrically based, fracture-matrix conductances (see Ho 1997, pp. 401-412, for more details).

2.4.3.3.1 Theory

Consider the flow of liquid, gas, and heat between a fracture and a matrix in an unsaturated domain (Figure 2-42). In dual-permeability models such as those used in TOUGH2 (Pruess 1991, pp. 28-32; 1987, p. 4-6), the fracture-matrix flow rates can be written as a function of state variables and properties associated with each material:

$$F_l = -\rho_l \frac{k_m k_{rl}}{\mu_l} A_l \frac{\Delta P_l}{d} \tag{2-25}$$

$$F_g = -\rho_g \frac{k_m k_{rg}}{\mu_g} A_g \frac{\Delta P_g}{d} \tag{2-26}$$

$$F_h = \lambda A_h \frac{\Delta T}{d} \tag{2-27}$$

where F_l, F_g, and F_h denote liquid, gas, and heat flow, respectively; ρ_l and ρ_g are densities of liquid and gas; k_m is the intrinsic matrix permeability; k_{rl} and k_{rg} are the relative permeabilities of the liquid and gas phases; A_l, A_g, and A_h are the areas available for liquid, gas, and heat flow; P_l and P_g are liquid and gas pressures; T is temperature; λ is thermal conductivity; and d is the nodal distance between fracture and matrix elements. In Equations (2-25) and (2-26) the liquid, gas, and heat flows depend on the hydraulic, pneumatic, and thermal conductances that all include a geometric conductance term, Γ, defined as follows:

$$\Gamma = \frac{A}{d} \tag{2-28}$$

The geometric area available for flow between a fracture and a matrix element, A, can be derived from the geometry of a uniform set of fractures and matrix-blocks lumped into a computational cell, which is often much larger than the actual matrix-block size (Figure 2-43). On the matrix-block scale (left sketch in Figure 2-43), the connection area between the fractures and matrix can be calculated as the length of the sides of the matrix-block in contact with fractures. The connection area between the fractures and matrix on the matrix-block scale, A', can then be written as follows assuming uniform matrix-blocks:

$$A' = N(D-b)^2 \tag{2-29}$$

where N is the number of matrix sides in contact with fractures (equal to four in the two-dimensional example in Figure 2-43), D is the fracture spacing, and b is the fracture aperture. The area in Equation (2-29) is then multiplied by the number of matrix-blocks that can occupy a single computational cell with volume, V, to yield the connection area, A, between the fracture and matrix element on the computational scale:

$$A = A' \frac{V}{D^3} \approx \frac{NV}{D} \tag{2-30}$$

The nodal distance between fracture and matrix elements, d, is estimated based on methods described in Zimmerman et al. (1993, pp. 2127-2137), Pruess (1983, pp. 6-8, 16-17), and Warren and Root (1963, pp. 245-255). When only one element is used to represent the matrix (as is often the case for DKMs), the nodal distance used in Equations (2-25)–(2-30) is determined so that the quasi-steady flux between the fracture and matrix element is comparable to the flux between a fracture and a continuous (rather than discrete) matrix unit. This nodal distance is given by Pruess (1983, pp. 6-8, 16-17) as follows for uniform matrix-blocks:

$$d = \frac{D-b}{N+4} \approx \frac{D}{N+4} \tag{2-31}$$

Table 2-36 gives the geometric fracture-matrix connection area and nodal distance for uniform one-, two-, and three-dimensional fracture sets. In this study, the fractures are assumed to be one dimensional (as opposed to two dimensional as shown in Figure 2-43).

Equations (2-30) and (2-31) define the geometric conductance term given in Equation (2-28). A major assumption in this formulation is that the entire geometric fracture-matrix connection area is available for flow. As demonstrated by Glass and Tidwell (1991, pp. 1-54) and Eaton et al. (1996, p. 4.1-4.14, 5.1-5.2), the actual area available for liquid flow between fractures and matrix can be much smaller than the geometric connection area. Heterogeneities at the pore-scale induce fingering processes that allow only a small fraction of the fracture surface to be wetted with liquid. In addition, flow-channeling at larger scales yields only a small fraction of the total number of fractures that are hydraulically active. The overall effect is a significant reduction in the geometric conductance term in Equation (2-28).

In past studies (Altman et al. 1996, pp. 76-81), a constant multiplier was used to reduce the geometric conductance term in simulations of unsaturated ambient flow at Yucca Mountain. The multiplier was used as a "fitting" parameter and its value was chosen so that simulated steady-state matrix liquid saturations matched observed data. However, modification of the geometric conductance term based on liquid flow cannot generally be applied to gas and heat flows as well. In addition, the fracture-matrix conductances should be functionally dependent on the flux or saturation in the fractures to accommodate changes in the hydraulic state of the fractures. Figure 2-44 shows a conceptual model of the changing geometric conductance for liquid flux as a result of the increased fracture-matrix wetted area from higher infiltration and a greater number of hydraulically active fractures.

In order to allow a significant reduction in liquid geometric conductance while honoring the gas and heat geometric conductances, the following model is proposed. The expressions for liquid and gas flows given by Equations (2-25) and (2-26) are multiplied by a fracture-matrix multiplier, $f(S_{up})$, which is a function of either the upstream liquid or upstream gas saturation. The expression for heat flow in Equation (2-27) is unaltered and retains full geometric conductance. Equations (2-25) and (2-26) can then be written as follows:

$$F_l = -\rho_l \frac{k_m k_{rl}}{\mu_g} \mathrm{A}_l \frac{\Delta P_l}{d} f(S_{up,l}) \tag{2-32}$$

$$F_g = -\rho_g \frac{k_m k_{rg}}{\mu_g} \mathrm{A}_g \frac{\Delta P_g}{d} f(S_{up,g}) \tag{2-33}$$

The functional dependence of the fracture-matrix multiplier on fracture saturation can take several forms:

$$f(S_{up}) = \begin{cases} C \\ S^{n}{}_{up} \\ k_r(S_{up}) \end{cases} \tag{2-34}$$

The first form of the fracture-matrix multiplier in Equation (2-34) is a constant, C, independent of saturation (this option is introduced here so that comparisons can be made to past studies that used a constant multiplier). The second form of the multiplier is the upstream saturation raised to a power, n. The final suggested form of the fracture-matrix multiplier is the upstream relative permeability. The liquid relative permeability, k_{rl}, is given by van Genuchten (1980, pp. 892-898) and Mualem (1976, pp. 513-522) as follows:

$$k_{rl} = \sqrt{\frac{S - S_r}{1 - S_r}} \left(1 - \left(1 - \left(\frac{S - S_r}{1 - S_r} \right)^{\frac{\beta}{\beta - 1}} \right)^{\frac{\beta - 1}{\beta}} \right)^2 \tag{2-35}$$

where β is a van Genuchten curve-fitting parameter and S_r is the residual saturation. Values of β have ranged from 1 to 3 in past studies of flow at Yucca Mountain (Bodvarsson and Bandurraga, 1996; Altman et al. 1996). Note that neither van Genuchten (1980, pp. 892-898) nor Mualem (1976, pp. 513-522) addresses nonwetting relative permeabilities in their papers. In this study, the gas relative permeability is assumed to be equal to one minus the liquid relative permeability.

The fracture relative permeability approximates the ratio of unsaturated flow (liquid or gas) in the fracture to saturated flow (liquid or gas) in the fracture if gravity forces dominate. The relative permeability of the fracture liquid therefore provides a conceivable measure of how much available wetted area is available for fracture-to-matrix liquid flow. The upstream relative permeability is specified in Equation (2-34) for generality. Figure 2-45 plots the fracture-matrix multiplier as a function of several different forms of saturation given in Equation (2-34). Note that for typical β values used in past studies for liquid relative permeability, the corresponding functional dependence of the multiplier on fracture liquid-saturation ranges from S^5_f to S^8_f. Several forms of the fracture-matrix multiplier are used in the next sections to assess which variables (e.g., liquid flow in fractures, matrix saturation, temperature) are sensitive to models of fracture-matrix conductances.

2.4.3.3.2 Discussion of Fracture-Matrix Interaction

A note should be made regarding the application of the fracture-matrix multipliers. Multipliers that are dependent on the hydraulic state of the system (e.g., upstream saturation and upstream relative-permeability multipliers) can be applied to all fluid phases. For example, if the multiplier is chosen to be upstream saturation, then the upstream *liquid* saturation is applied to fracture-matrix liquid flow while the upstream *gas* saturation is applied to fracture-matrix gas flow. However, the use of a constant multiplier should be limited to fluid phases that can be calibrated to available data. For example, in Case 4, a constant multiplier was used to calibrate the model with liquid-saturation data. Therefore, the constant multiplier should have been applied only to fracture-matrix liquid flow (in this study, it was applied to liquid, gas, and heat flows to make comparisons with previous studies). Rather than using this constant for the gas-phase flow as well, a more reasonable assumption for the gas-phase multiplier is $1-C$.

Using constant multiplier during transient flow also contains caveats that were not clearly illustrated in this study. If C is nearly 1 (indicating fully wetted fracture surfaces), the gas-phase conductance multiplier ($1-C$) would be very small. If heating and drying occurred, one would expect the fracture-matrix gas-phase conductance to increase. While the hydraulically dependent multipliers (upstream saturation and upstream relative permeability) would correctly account for this transient behavior, the constant multipliers would yield inaccurate values when the available wetted area between fractures and matrix had changed from their original calibrated values. The impact of these inaccuracies on specific processes such as fracture flow or matrix saturation is uncertain and likely will depend on the nature and processes of each particular system.

Because of the uncertainty in fracture-matrix interactions in unsaturated fracture media, a fracture-matrix conductance scaling factor can be used as a fitting parameter to calibrate the model to available data. Constant multipliers, which were determined by calibrating the model to saturation data, and upstream relative permeability multipliers yielded the best matches to data in Ho (1997, p. 409) and produced similar results during ambient and heated conditions.

2.4.3.4 Analysis of Perched Water

Incorporation of perched water data is an important aspect of the UZ-flow-model calibration. The presence of perched-water bodies implies that vertical water fluxes locally exceed the saturated hydraulic conductivities of the perching layers. In order to capture the perched-water phenomena, the UZ-flow model must have a representative geologic/conceptual/trapping model, fracture/matrix properties, and sufficient net infiltration. The resulting model should reproduce hydraulic responses in pumping tests and remain consistent with geochemical data and the areal extent of the perched body. This section summarizes the perched-water model calibration efforts of FY-97 (Bodvarsson et al. 1997, Chapter 13), focusing on geology and hydrology.

Perched water can be defined as a SZ not directly connected to the static water table (Freeze and Cherry 1979). Two criteria must be met for the model to accurately reproduce perched water at Yucca Mountain. The first is that water saturation within a perched-water zone must be sufficiently high to initiate substantial fracture flow (if any fractures are present). The second is that water pressure within the perched-water volume must obtain values higher than the static atmospheric-gas pressure that would be expected at the same elevation. Under these conditions, water will flow freely into a borehole intersecting a perched-water body. Perched water may accumulate where large contrasts in hydraulic conductivity exist between adjacent formation units, where a permeable layer overlies a relatively impermeable layer, or where a well-connected fractured unit overlies a locally unfractured or poorly connected fractured unit. Relative fracture density and fracture permeability have a strong influence on the accumulation of perched water (Burger and Scofield 1994, p. 250). Perched water may also exist against a fault along a dipping horizontal plane if the fault acts as a barrier to downdip water flow.

One of the implications of an existing perched-water body is that the flow path may not be vertical through the UZ to the water table, but rather the water may be diverted laterally to a fault zone or other type of higher permeability channel in order to reach the water table. As a result, a nonuniform recharge rate to the water table is expected. This has important implications for waste isolations at Yucca Mountain. Existence of perched-water zones along the base of the Topopah Spring welded unit implies that water may partially bypass the underlying zeolitic unit, and consequently some radionuclides may not be retarded by the highly sorbing zeolites.

Conceptual Model

The genesis of the perched-water bodies at Yucca Mountain is much debated. During the Pleistocene, pluvial lakes covered many currently dry salt flats and lake beds, decreasing chloride deposition rates at the land surface (Fabryka-Martin et al. 1996, pp. 6-9). Low chloride concentrations in perched-water bodies indicate that much of the recharge to perched bodies at Yucca Mountain may have occurred during this time. Carbon 14 ages, however, do not support this argument, but rather indicate apparent ages of 3,000 to 7,000 years (Yang et al. 1996, pp. 12-39, 55). Furthermore, stable isotope values for $\delta^{18}O$ and δD also support post-glacial recharge (Yang et al. 1996). It therefore seems unlikely that perched water at Yucca Mountain is a remnant of past climate conditions.

Several possible conceptual models could explain the low chloride content of the perched water bodies. Because the chloride content of the matrix water in the PTn is high, all alternative conceptual models depend on flow circumventing the matrix of this unit. For example, it is possible that flow paths from Solitario Cañyon or from the area near G-2 transmit flux under the PTn to the perched bodies. Another alternative explanation is that the water was recharged from the surface through fast-pathway fracture flow, with little interaction with the matrix. This hypothesis was favored by Yang et al. (1996) in their report on UZ hydrochemistry. Further evidence supporting fast-fracture recharge may come in the future from strontium isotopic data.

Identification of perched-water zones at Yucca Mountain is complicated by the lack of field data and by uncertainties as to the exact location of the phreatic surface in some areas. For example, it has been proposed in the past that the water table in the vicinity of Boreholes G-2 and WT-6 (located about 1.5 km northeast to G-2) may be as much as 300 m higher than the elevation under the proposed repository (Ervin et al. 1995, pp. 1-15). Currently, however, evidence appears to favor the theory that this elevated potentiometric surface represents an extensive perched-water body. This evidence includes a small but consistent decrease in the measured elevation of the potentiometric surface since the drilling of G-2 in the mid-1980s, and the presence of unsaturated core samples below the apparent water table (Chapter 13 in Bodvarsson et al. 1997) in the borehole. Most persuasively, recent pump-tests at G-2 have resulted in an apparent long-term decrease in the elevation of the water table; 236 days after cessation of pumping, the potentiometric surface did not fully recover to the original level, and remained approximately 0.5 m below the pre-pumping level.

Another complicating factor in identifying perched water is that the relatively uniform water-level elevations measured in the vicinity of the proposed repository may actually represent the potentiometric surface of a confined aquifer. This theory is supported by less-than-saturated core recovered in several areas below the supposed surface of the water table, and by experience gained in advancing several boreholes into the SZ. For example, during the drilling of UZ-16, core recovered below the projected potentiometric surface was found to be unsaturated; however, when the borehole encountered fractures in apparent hydraulic communication with the SZ, the potentiometric surface rebounded to its projected elevation (Chapter 13 in Bodvarsson et al. 1997).

Perched-water bodies and areas of wet-core recovery from Yucca Mountain boreholes are generally detected in zones overlying geologic units of decreased fracture and/or matrix permeability, such as the basal vitrophyre of the Topopah Spring (Tptpv3, basal vitrophyre of the crystal-poor vitric unit). Borehole fracture frequencies for the Tptpv3 unit are very high relative to the other geologic formations at Yucca Mountain (Bodvarsson et al. 1997, Chapter 7), while matrix permeabilities are relatively low (Flint 1998, p. 44). Borehole log data indicate that the fractures in the Tptpv3 serve as the main pathways for water flow through the unit, causing alteration to low permeability minerals. The resulting increase in volume of the altered minerals may effectively block flow through the fractures (Rousseau et al. 1998).

Current information suggests that this is an important perching mechanism for the majority of perched-water occurrences (those at UZ-14, SD-9, SD-12, and NRG-7a). Additionally, for SD-9 and NRG-7a, the vitric units underlying the Tptpv3 have also been extensively altered to low-permeability zeolites, which would aid in the perching. An exception to this general trend is seen at SD-7, where a smaller, probably isolated body is perched on the low-permeability bedded tuffs between the Calico Hills and Prow Pass tuffs. Also, if the water body at G-2 is perched, then the perching occurs in the zeolitic CHn hydrogeologic unit below the basal vitrophyre of the TSw.

In the present study, perched water was assumed to follow the conceptual model as outlined above. The main perched-water body (surrounding UZ-14, SD-9 and NRG-7a) was assumed to be hydraulically connected; to exist primarily within the fractured, welded base of the TSw lower nonlithophysal zone; and to be underlain by the crystal-poor vitric unit (basal vitrophyre) where fractures filled with low permeability products of alteration block flow paths. The smaller, probably isolated, perched-water bodies (at SD-7 and SD-12) are believed to be perched as a result of juxtaposition of different permeability units at the Ghost Dance Fault.

Analysis

Previous modeling studies of perched water at Yucca Mountain were reported by Bodvarsson and Bandurraga (1996). In the more recent FY-97 work, two boreholes (G-2 and SD-12) were included in addition to the boreholes considered in the 1996 report, and a series of three-dimensional simulations were conducted using the TOUGH2 code. The model incorporated perched-water observation data available from Boreholes USW UZ-14, NRG-7a, SD-7, SD-9, G-2, and SD-12. The UZ flow model incorporated the observed perched-water data and used the generalized ECM to account for fracture and matrix interactions. The GECM was expected to accurately describe perched-water conditions at Yucca Mountain because water flow and distributions at perched-water zones were likely to be present at steady-state or quasi-steady-state conditions. The current perched-water bodies, as indicated by the water ages from geochemical data, have existed for thousands of years. Under such conditions, the ECM formulation was shown to be accurate for treatment of fracture/matrix interactions (Bodvarsson et al. (1997, Chapter 5). It should be noted, however, that the conceptual model used in TSPA-VA is a DKM. Similar calibration procedures to the ones described here were also used to match perched-water data for the DKM simulations (see Section 2.5).

The present-day infiltration map (Flint et al. 1996) was employed in this work to describe the distributed net infiltration condition at the land surface, and both steady-state and past transient-infiltration scenarios were considered. The work performed can be summarized as follows:

A. The observed perched-water data from six boreholes were incorporated into a three-dimensional perched water, UZ flow model.

B. The three-dimensional perched-water model was calibrated using observed perched-water locations and moisture data from perched-water boreholes. Observed data were compared with the predicted perched-water locations, liquid-saturation and water potential data, and reasonable agreement was obtained. The spatial distributions of perched-water bodies at Yucca Mountain were modeled.

C. Three numerical simulations of pumping tests were conducted for perched-water bodies encountered at Boreholes UZ-14 and G-2, respectively, and the simulated water levels of pumping and recovery periods were in good agreement with actual pumping data. Based on the pumping test analysis, the minimum volumes of the perched-water bodies around UZ-14 and G-2 were estimated.

D. Perched-water ages were estimated using groundwater travel times through the fracture/matrix system, and the results are in reasonable agreement with residence ages determined from isotopic studies.

E. An assumed scenario of the past high-infiltration rates was simulated and the impacts on perched-water level changes were predicted.

Summary and Conclusions

Chapter 13 of Bodvarsson et al. (1997) details how the field-observed, perched-water data at the Yucca Mountain site were compiled, analyzed, and incorporated into the three-dimensional UZ flow model. A conceptual model of occurrences of perched water was discussed, and a series of comprehensive computer modeling studies on perched water at the site was completed. A three-dimensional UZ perched-water flow model was then developed to investigate the perched-water phenomena at Yucca Mountain.

Perched-water data observed in six boreholes were discussed and used to calibrate the three-dimensional model in reproducing the water-perching conditions in the UZ of the mountain. Geochemical data have been considered in the conceptual model of the perched water, and a near-surface model for chloride balance in Yucca Mountain was described. The three-dimensional, steady-state, and transient simulations have been conducted using the updated, distributed-infiltration map (Flint et al. 1996; CRWMS M&O 1998. *Yucca Mountain Site Description*, Section 5.3.4.1) as the surface net infiltration condition. A three-dimensional perched-water model was constructed and used to investigate the effects of fracture and matrix permeability variations of the welded and nonwelded tuffs near the perched-water zones. The calibrated parameters of rock properties in this study were fracture and matrix permeabilities, capillary functions and residual-gas saturations within the perched-water zones. Adjusted permeabilities were within the range of the observed or laboratory-tested values. The key factors in creating a perched-water zone at the UZ system of Yucca Mountain are (1) an existing water-perching geologic structure underlain and surrounded by low-permeability zones; (2) weak capillary suctions under high-saturation conditions within and near perched-water zones; and (3) sufficient water-infiltration rates.

The steady-state simulation results of this modeling study were in agreement with the observed perched-water data, including water-saturation and potential profiles and perched-water elevations. The three-dimensional model reproduces the water-perching conditions as observed from the boreholes. The three perched-water zones around (UZ-1/14, SD-9, NRG-7a and G2); (SD-7); and (SD-12) were estimated for volumes and spatial extent and are shown using two-dimensional and three-dimensional plots from the simulation results.

Transient numerical pumping tests were performed using the three-dimensional model for Boreholes UZ-14 and G-2. The numerical pumping test results matched the observed water-level data from pumping to recovery at both boreholes. The perched-water volume around UZ-1/14 was estimated to be about one million cubic meters. At G-2, a much larger perched-water body of 100 million cubic meters was estimated from the pumping data analysis.

In an effort to further calibrate the three-dimensional perched-water model, a particle-tracking analysis was performed to estimate the groundwater travel times from the land surface. The water ages derived from particles traveling through the fracture/matrix system were in reasonable agreement with those estimated from ^{14}C residence times. In addition, the three-dimensional, steady-state simulation results also showed that large lateral flow may exist within the PTn and along the zeolitic interfaces in the CHn above the perched-water body.

The effects of historic high infiltration rates were investigated using an assumed 1,000-year period of high infiltration, taking place 10,000 years ago. It was found that the perched-water levels at the boreholes having perched water may be increased by several meters, because the infiltration events are high. This analysis indicated that it will take from 1,000 to 3,000 years for the UZ system to return to a steady-state, equilibrium condition after a large, prolonged, infiltration event.

2.4.3.5 Geochemical Analyses

The following geochemical analyses were performed by Bodvarsson et al. (1997, Chapter 15). They are included to further demonstrate the efforts made in calibrating the LBNL flow model to geochemical data. These analyses also provide methods of developing bounds and ranges for percolation flux and infiltration. The reader is referred to Chapters 14-18 of Bodvarsson et al. (1997) for more details.

2.4.3.5.1 Modeling the Chloride Geochemistry in the UZ

Conceptual models for the spatial and temporal variations in chloride chemistry at Yucca Mountain were implemented in a three-dimensional submodel and the full three-dimensional LBNL UZ site-scale model (Chapter 15 of Bodvarsson et al. 1997). The spatial variation in surface chloride concentrations was calculated using maps of precipitation and infiltration for the current climatic conditions and for the last glacial maximum (about 5.5 times higher mean infiltration), combined with measured concentrations in precipitation and mean chloride surface fluxes. This study suggested that the current mean infiltration rate (~4.9 mm/yr) is probably a maximum value for the repository at Yucca Mountain. Depending on the total chloride flux at the surface, the mean infiltration may be as low as 1 mm/yr. Analysis of the chloride data and the modeling showed that waters as old as the last glacial maximum, or earlier, could be present at shallow depths in the PTn, and certainly in the Topopah Spring welded tuff, predominately under alluvial channels with little or no infiltration. Perched-water compositions were closely matched using the 21 kA precipitation and infiltration, although UZ-14 may have had a slightly larger proportion of more chloride-rich modern water. The three-dimensional simulations showed that there was significant mixing of high-chloride water under alluvial channels with low-chloride water flowing laterally in the Calico Hills, resulting in mixed compositions at depth. Comparisons to pore-salt measurements in the ESF showed that the variability may be explained by predominantly vertical flow under high- and low-infiltration regions. Some lateral flow along the PTn up to about 100 m or so may also be expected. The high chloride concentrations in pore waters at the Ghost Dance Fault and under other low-lying structural features may strongly mask any "bomb-pulse" ^{36}Cl entering the subsurface in those locations. This was further supported by the finding of "bomb-pulse" tritium in samples collected in and near the Ghost Dance Fault (Chapter 15 of Bodvarsson et al. 1997).

2.4.3.5.2 Modeling the Strontium Geochemistry and Isotopic Ratio in the Unsaturated Zone

The geochemistry of strontium in pore waters at Yucca Mountain can yield important constraints on the flow regime and percolation fluxes to the repository in the UZ. Strontium concentrations are related to the infiltration rate (through evaporation), the dissolution of minerals in surface deposits, reaction with minerals or glass in the tuffs, precipitation of calcite, and exchange with clays and zeolites. Strontium isotopic ratios in pore waters are affected directly through mineral dissolution and ion exchange, and indirectly through the change in total Sr by precipitation along flow paths. Assuming that flow is predominantly vertical, the Sr isotopic ratio ($^{87}Sr/^{86}Sr$) in pore waters can be interpreted in terms of values of "R/Svf," where R is the reaction rate (dissolution rate) of the rock material, and Svf is the percolation flux (rate), in terms of mm/yr (v is the bulk fluid velocity, f is the bulk porosity, and S is liquid saturation). Using the values for R of ca. $5 \pm 3 \times 10^{-9}$ yr^{-1} deduced from fractured basalt systems elsewhere, and a pore-fluid Sr concentration in the range 0.5 to 1.0 mg/L, the percolation flux in the Topopah Spring welded tuff for Borehole SD-7 was estimated to be between 0.5 and 5 mm/yr, compared to the calculated local surface infiltration rate of 3.6 mm/yr (Chapter 17 of Bodvarsson et al. 1997). The effects of rate-limited dissolution and precipitation on the concentration of a solute were incorporated into a module for TOUGH2, as were dispersion, radioactive decay, and linear equilibrium adsorption already treated in the T2R3D module (Wu et al. 1996, pp. 1-52). Preliminary results of one-dimensional dual-permeability modeling suggested that an increased reaction rate in the Paintbrush bedded tuffs can yield a significant shift in the Sr concentrations, similar to the pattern observed in the $^{87}Sr/^{86}Sr$ in SD-7.

2.4.3.5.3 Analysis of ^{14}C Data Using the UZ Model

The study of ^{14}C as a tracer of total carbon behavior and transport can provide a useful tool for constraining (and possible determination of) percolation rates through Yucca Mountain (Chapter 18 of Bodvarsson et al. 1997). The current data availability on ^{14}C concentrations in the gas phase, the pore water, perched-water tables, groundwater, and secondary calcite deposits is limited. There are reasons to believe that a large portion of the perched-water-table data on ^{14}C from the UZ-14 well are compromised as a result of contamination by drilling fluids.

A review of the models used to simulate the ^{14}C fate and transport shows that they range from simple one-dimensional gas-diffusion models to sophisticated multi-dimensional, multi-component flow and transport simulators with radioactive decay, interphase partitioning and chemical speciation under local equilibrium conditions. Most of these models can predict ^{14}C concentrations with depth (one-dimensional) in the gas phase in good agreement with observations, using conceptual underpinnings that may be fundamentally different. The complexity of the processes involved in the fate and transport of total carbon with ^{14}C necessitates the use of the more sophisticated models, e.g., FEHM (Zyvoloski et al. 1996, pp. 93-115) and TOUGH2 (Pruess 1991, pp. 28-32) with EOS7R (Oldenburg and Pruess 1995, pp. 5-18). Neither of these models can currently handle kinetically-controlled reactions. FEHM has phase partitioning and speciation capabilities, but only in the equivalent continuum mode (its dual permeability mode is limited to flow and transport). TOUGH2 has phase partitioning in both the equivalent continuum and the MINC mode (of which dual permeability is an option), but currently lacks chemical-speciation capabilities.

Using TOUGH2/EOS7R, a very good match between simulation results and ^{14}C observations at the UZ-1/UZ-14 wells was obtained (Chapter 18 of Bodvarsson et al. 1997). Flow and transport through the one-dimensional domain was nonisothermal and involved a dual-permeability system. Using the optimization algorithm of Thomas and Hellums (1972, pp. 508-514), the percolation rate corresponding to the minimization of residuals between predictions and observations was estimated at 4.2 mm/yr. This is in good agreement with the 4.9 mm/yr used in matching the saturation distribution in the UZ-1/UZ-14 wells. The same simulation predicted a temperature distribution that was in very good agreement with measurements.

2.4.3.6 Weighting Schemes for UZ Flow

During the course of the UZ flow sensitivity analyses, it was discovered that the choice of the numerically implemented weighting scheme for the absolute permeability and relative permeability was a significant issue that could affect transport times below the repository. Specifically, large amounts of water percolating through the high-permeability vitric matrix elements could either be diverted into the vitric fracture elements or allowed to flow into the low-permeability zeolitic matrix elements, depending on the weighting scheme used for the hydraulic conductivity between adjacent elements in the flow simulations. The discrepancy appeared in comparison studies between TOUGH2, which typically uses full upstream weighting of the absolute and relative permeabilities, and FEHM, which typically uses harmonic weighting of the absolute permeability and upstream weighting of the relative permeability. Full upstream weighting was found to over-predict the conductivity between the high-permeability vitric matrix overlying the low-permeability zeolitic matrix. As a result, a significant amount of water would enter the zeolitic-matrix from the vitric matrix, sometimes surpassing the saturated conductivity of the zeolitic-matrix element. On the other hand, the combined harmonic weighting of the absolute permeability with the upstream weighting of the relative permeability was shown to possibly under-predict the conductivity between the two units. The absolute permeability was weighted toward the low-permeability zeolitic material, and the relative permeability of the upstream vitric layer was lower than the nearly saturated zeolitic matrix element below. As a result, a compromise was proposed among participants to modify the upstream weighting scheme so that the low conductivity of the zeolitic-matrix units could be taken into account at interfaces where a vitric-matrix element overlies a zeolitic-matrix element. At those connection pairs, a downstream weighting of absolute and relative permeabilities is used.

To test and compare the weighting schemes, a two-dimensional simulation of UZ flow at Yucca Mountain was performed. Figure 2-46 shows the two-dimensional model, which corresponds to an east-west cross-section of Yucca Mountain at a northing coordinate of 233,400 m. The domain was bounded on the west and east by the Solitario Canyon and Ghost Dance faults, respectively. The faults were conceptualized to be capillary barriers so that any lateral liquid flow was diverted downward at these boundaries. The bottom of the domain corresponded to the water table and was maintained at a constant saturation of one. Infiltration was introduced at a prescribed, spatially varying rate along the top row of fracture elements. The DKM was used with prescribed reduction factors for fracture/matrix interaction to account for isolated flow paths and liquid channeling on fracture surfaces. The mesh consisted of a total of 5,632 fracture and matrix elements, and the hydrologic properties and infiltration distribution were taken from LBNL (DTN: LB971100001254.002).

The EOS9 module (Richards' solution) of TOUGH2 (SNL QA Version 3.1.1) was used to generate liquid-flow fields in the model. To facilitate particle tracking in the TOUGH2-generated flow fields using FEHM, a post-processor was written to reformat the TOUGH2 output into FEHM-readable files (see next section). These processed files were then read by FEHM, and radionuclide mass-flux and cumulative-breakthrough curves were generated using the particle-tracking solution. In the particle-tracking solution used in this study, 500,000 particles representing ^{237}Np were released instantaneously at the potential repository horizon at t=0. The diffusion coefficient was set equal to $1x10^{-11}$ m^2/s, and a constant sorption coefficient, K_d, of 2.5 cc/g was used for ^{237}Np in the zeolitic units (zero elsewhere). Hydrodynamic dispersion was neglected (in the context of not including a physical dispervisity value in the model). Dispersion caused by the coarseness of the numerical grid may influence the results, but it should be the same in all simulations using the same grid.

Results

The mass flux of ^{237}Np at the water table as a function of time is shown in Figure 2-47 for the three different weighting schemes used in the two-dimensional TOUGH2 flow simulations: 1) full upstream (upstream absolute and relative permeabilities), 2) harmonic absolute permeability (with upstream relative permeability), and 3) modified upstream (with downstream weighting of absolute and relative permeabilities at connections where a vitric matrix overlies a zeolitic matrix). Two peaks are evident in all the simulated mass fluxes as a result of disparate travel times of ^{237}Np through the fracture and matrix continua.

Significant differences in the initial arrival time at the water table can be attributed to the different flow behavior at the interface of the vitric- and zeolitic-matrix elements resulting from the different weighting schemes. (Note: sensitivity studies revealed that refinement of the mesh was not the source of the discrepancy.) In the full upstream-weighting simulation, large amounts of water could flow downward from the high-permeability vitric matrix to the low-permeability zeolitic matrix below, even though the permeability decreased by up to four orders of magnitude. In fact, because of the upstream weighting of the hydraulic conductivity, the rate of flow entering the zeolitic matrix could exceed the saturated conductivity of the zeolitic matrix material, which is physically unrealistic. The increased flow through the zeolitic matrix allowed the ^{237}Np to be sorbed and delayed the breakthrough at the water table. Although some of this water was eventually forced into the zeolitic-fracture elements (denoted by the first ^{237}Np peak in Figure 2-47), a significant amount of ^{237}Np was carried through the matrix, as evidenced by the second ^{237}Np peak in Figure 2-47.

In contrast, the harmonic absolute permeability weighting scheme resulted in a much earlier breakthrough of ^{237}Np at the water table. This scheme yielded a much lower hydraulic conductivity between vitric-matrix elements overlying zeolitic-matrix elements relative to the full upstream weighting scheme. As a result, water flow was diverted around the zeolitic matrix and into the vitric-fracture elements, and the unrealistic transport time-delay for ^{237}Np is eliminated. However, the harmonic absolute permeability was weighted towards the low absolute permeability of the zeolitic matrix, and the upstream relative permeability of the vitric matrix was typically much less than the relative permeability of the nearly saturated zeolitic matrix. Therefore, the resulting product was less than the actual conductivity of the zeolitic matrix, and potentially too much flow may have been diverted away from the zeolitic matrix.

The results of the modified upstream scheme showed that the initial ^{237}Np breakthrough was similar to the results of the harmonic weighting scheme (Figure 2-47), indicating a significant diversion of flow into the vitric fractures; the second peak is more pronounced, indicating increased transport through the zeolitic matrix. This behavior is better illustrated in Figure 2-48, which shows a plot of the cumulative-travel-time distributions for the different weighting schemes. The first plateau of the cumulative-breakthrough curve was proportional to the mass flux reaching the water table under a constant-release scenario. The modified weighting scheme yielded significantly lower mass-flux values than the harmonic case within the first 10,000 years, indicating less flow through the fractures, but the arrival times were not shifted to longer values as in the upstream case. This behavior is a compromise between the extreme behaviors of the other two weighting schemes and is believed to be more defensible. As a result, the modified upstream method was used to generate flow fields for the TSPA-VA calculations.

2.4.3.7 Interface Between UZ Flow and UZ Transport

TOUGH2 (Pruess 1991, pp. 28-32) and FEHM (Zyvoloski et al. 1996, pp. 93-115) are two prominent codes for evaluating flow and transport in the UZ for PAs of the potential high-level nuclear waste repository at Yucca Mountain, Nevada. The application of TOUGH2 has focused on site-scale UZ hydrology (Bodvarsson et al. 1997, Chapter 14), while the use of FEHM has focused on fluid flow and radionuclide transport (Robinson et al. 1997) at Yucca Mountain. Both UZ hydrology and radionuclide transport are critical components in performance-assessment calculations, and methods of coupling these components were investigated for TSPA-VA.

Two methods were considered to transfer the UZ-flow results to the UZ-radionuclide-transport model, which was chosen to be the particle-tracking method in the computer program FEHM (Zyvoloski et al. 1996): (1) use the UZ-flow fields calculated by TOUGH2 directly as input to the FEHM particle tracker, or (2) take the stratigraphy and calibrated hydrologic parameters and use them as inputs to a combined flow and transport calculation within FEHM. The primary advantages of the first option are that preservation of the UZ-flow calibration is assured, and it is not necessary to recalculate the flow and recheck the calibration. The primary advantages of the second option are that the FEHM particle tracker is already set up to use flow fields calculated by FEHM (the first option requires development of a linking program to take TOUGH2 output and generate FEHM input), and there is additional flexibility to refine the computational grid to make the transport calculations more accurate. Testing was done to compare these options, (Ho et al. 1998; currently available at http://www.nwer.sandia.gov/ymp/comparison/options.html, 2/24/98), and although they both appeared to be viable, the advantages of the first option were thought to outweigh those of the second option. Thus, the first option (flow fields calculated with TOUGH2, radionuclide transport calculated with FEHM), has been implemented in TSPA-VA.

The particle-tracking method used in FEHM is a cell-based model in which particles are routed from grid block to grid block in a manner that preserves the overall residence time through any portion of the model and probabilistically reproduces the migration of a solute through the domain (Robinson et al. 1997). The requirement for the method is that the flow calculation be based on a control volume in which fluid-flow rates into and out of each cell are computed. Since TOUGH2 is an integrated, finite-difference code and FEHM employs a control-volume, finite-element technique, the two codes are compatible from the standpoint of implementation of the particle-tracking technique. The required inputs for FEHM to use an externally developed flow field are: (1) grid-connectivity information and cell volumes; (2) fluid-state variables for computing density, fluid saturation, and rock porosity at each grid point; (3) internodal fluid-mass-flow rate for every connection in the numerical grid; and (4) fluid source and sink-flow rates for each grid block.

A post-processor was written to convert the TOUGH2 DKM flow fields into FEHM-readable files. The processor maps several pieces of relevant information from the TOUGH2 output files to input files for the FEHM particle tracker: mesh information, properties, and mass flow between elements/nodes. The finite-volume element-based mesh of TOUGH2 is mapped onto a nodal-based grid used by FEHM. Both fracture and matrix elements are retained for particle tracking. Relevant fracture and matrix properties for the particle tracker (e.g., liquid saturations and porosities) are also mapped from the TOUGH2 elements to the corresponding FEHM nodes. Finally, the mass flows into and out of each TOUGH2 element, including fracture-matrix interactions, are mapped to a FEHM restart file. The code is currently being qualified under SNL QAIP 19-1.

2.4.3.8 Grid and Model Domain for LBNL Three-Dimensional Site-Scale UZ Flow Model

Design of the LBNL three-dimensional grids (see Chapter 4 of Bodvarsson et al. 1997, for full details) was based on the non-Q LBNL geological model and non-Q geological framework model, both showing consistency over the potential repository area and excellent agreement with borehole data. Although most of the grid generation was carried using the non-Q code, AMESH, the methods employed followed documented and well-established geometrical principles (Palagi 1992, pp. 15-79) and were similar to the mesh generation method used in the Q code TOUGH2 (Pruess 1991, pp. 28-32).

The three-dimensional numerical grids were designed in two steps: (1) using all available surface information to create a horizontal, two-dimensional grid, and (2) integrating data from isopach maps of hydrogeological units to vertically develop the horizontal grid between the ground surface and the water table. This model was a further update of the existing LBNL three-dimensional UZ model first developed by Wittwer et al. (1992, pp. 263-271), which was later updated in 1996 (Bodvarsson and Bandurraga 1996). The development of this new model, like the old one, started with the definition of the grid block centers that defined a single two-dimensional horizontal grid to use in all the three-dimensional vertical layer sections. After all the nodal points had been located, a numerical grid generator AMESH was used to develop the two-dimensional horizontal grid. These two-dimensional horizontal grids and the sub-layering criteria were used to develop a new three-dimensional numerical grid of the UZ at Yucca Mountain.

New boundaries for the site-scale model were developed as an update to the 1996 three-dimensional LBNL UZ model. These boundaries were based on revised fault maps, the observed shift in water level across the Solitario Canyon, the new infiltration and alluvium thickness maps, the observed pneumatic signals (Ahlers et al. 1996) during the construction of the ESF Tunnel, and the requirements for thermal loading studies. The new boundaries take into account the extensive high-gradient SZ to the north of G-2 and explicitly included the Solitario Canyon Fault in the west, by extending the model boundary to about 1 km west of Solitario Canyon fault. The Bow Ridge fault forms the eastern boundary. The model extends from G-3 in the south to about 1.5 km north of G-2 in the north. These boundaries enclose most of the existing and planned hydrology wells and the wells in which extensive moisture tension data and lithology are used as calibration points for formation properties. The 1997 site-scale model was based on the fault map that provided explicit offsets on Solitario Canyon Fault, Ghost Dance Fault, Ironridge, and the Dune Wash Fault, defined by the base of the Tiva Canyon.

One primary objective in the selection of grid boundaries was to minimize boundary effects resulting from thermal loading at the repository horizon, while investigating the influence of the major faults on the hydrological and thermal-hydrological response of the UZ at ambient conditions and during thermal loading. The modeled area covers nearly 43 km^2 and is bounded by Bow Ridge fault on the east; extends 1 km west of Solitario Canyon; is bounded by the plateau of high pressure gradient about 1.5 km north of G-2; and extends about 1 km south of the ESF south ramp. In this grid, the "East Block Repository" area is modeled as a locally refined area with an average grid of 100 × 100 m and accounts for proposed extension of the potential repository to the north. The resulting two-dimensional grid contains a maximum of 1,470 aerial grid-block nodes in each layer. The two-dimensional grid extends about 1 km west of the Solitario Canyon in order to explicitly model both the Solitario Canyon fault and its associated Iron Ridge fault branch to the south. Explicit modeling of the area west of the Solitario Canyon also allows for specification of the 40-m shift in the water table west of this fault. This grid was used to perform general site-scale UZ modeling and for detailed studies related to thermal loading of the repository.

2.4.3.8.1 Criteria for Two-Dimensional Grids

The following criteria were used for the choice of grid-block centers in the two-dimensional grid described above.

A. Locations of existing or planned boreholes were used as centers, subject to minimum spacing of 100 m between grid blocks. Priority was given to wells that were used for model calibration (e.g., UZ, SD, NRG, SRG, WT, and RF Boreholes).

B. Nodes at an average spacing of 100 m were placed along the trace of the ESF. Where any overlap occurred with existing or planned boreholes, the ESF block center was used.

C. Locally refined grid-block centers were placed at a spacing of 100 m and aligned in the direction of the proposed repository drifts. Where an overlap occurred with the planned or existing boreholes or the trace of fault, the refined grid-block center (repository-block center) was used.

D. Elements were aligned along the trace of all the major faults to be explicitly modeled, ensuring that all elements along the faults have interfaces with only two neighboring fault elements (i.e., "back-to-back connection"). In addition to this back-to-back connection, the elements were spaced so that fault elements in two neighbor faults were separated by at least a single row of nonfault blocks. This was necessary in order to uniquely compute the layer offsets across the faults.

E. Nodes were also distributed so that key features of the distributed infiltration could be accurately modeled, based on the infiltration maps used in this study.

F. Nodes were also aligned along the trace of Drillhole Wash Fault, Severe and Pagany Wash, as well as Yucca Wash, in order to allow for assignment of individual properties along them if required.

2.4.3.8.2 Development of the Three-Dimensional Numerical Grids

The three-dimensional grids were developed on the basis of the two-dimensional grids and the spatial distribution of main hydrogeological units. These units are the welded members (Tiva Canyon and Topopah Spring) and the nonwelded members (Paintbrush and Calico Hills). A fixed number of vertical layers were chosen for each unit, allowing for a lateral continuity of the layers. The new isopachs provide explicit layer thickness for all the sublayers in the Paintbrush (five layers) and Calico Hills (ten layers).

The layers in the UZ model correspond to the major hydrogeologic units and alteration zones as discussed by Bodvarsson et al. (1997, Chapter 3). For the TOUGH2 DKM with one matrix and one fracture block per model layer, the block designations replace the first number in the label for the layers representing the TCw, TSw, and PTn by M (for Matrix block) or F (for Fracture block). Therefore, a one-dimensional model grid has two blocks for UZ model layer tcw11, i.e., block tcwM1 and block tcwF1. For the model layers below the TSw, the ECM layer name is altered to include a capital M or F designating a matrix or fracture block. For example, the vitric ECM layer designated ch1vc has two blocks labeled ch1Mv and ch1Fv in the DKM.

The top of the model was represented by the top of the Tiva Canyon (i.e., ground surface minus the thickness of the alluvium). This approach allowed direct application of the net infiltration data to the top nodes in the three-dimensional model. This Tiva Canyon unit was divided into three sub-layers, in which the thickness of the base of the Tiva Canyon was set at a maximum of 6.0 m and the remaining Tiva Canyon subdivided equally into two units. Calico Hills was represented by four sublayers in the Calico Hills unit and two sublayers (a vitric and zeolitic unit) in each of the lower Prow Pass, Bullfrog, and Tram hydrogeologic units. The Topopah Spring is subdivided into seven model layers representing seven explicit formations. These hydrogeological sub-layers represent, as closely as possible, lithological variations within the main units.

The AMESH grid generator was adapted to generate the three-dimensional grid. In order to take into account the fault offsets within the columns of grid blocks located along the fault traces, the generation of the numerical grid was performed in two steps; dealing first with all grid blocks except those including offsets, then taking care of grid blocks with offsets (the fault grid blocks). The grids for nonfault and fault sections were then combined to obtain the three-dimensional numerical grid for the whole site-scale model area. Two separate grid-generation schemes were necessary because in this scheme, each two-dimensional vertical element was split into two or more parts in proportion to the vertical interface area between adjacent fault and nonfault nodes in order to generate connections across different hydrogeological units or layer offsets.

2.4.3.8.3 Development of Grid Blocks with and without Fault Offsets

Generating the grid for all the grid blocks outside the fault zones involved obtaining the correct volumes and interfaces for the grid blocks adjacent to the faults. The modeled area was divided into five blocks. Each of those blocks was delimited by faults and/or model boundaries. The offsets across the faults were defined by the elevation of the base of the Tiva Canyon in neighboring blocks. The first block consists of all grid blocks located west of Solitario Canyon fault. The second block is pinched between Solitario Canyon and Iron Ridge Faults. The third block is bounded by Solitario Canyon and Iron Ridge Faults in the west, and the Ghost Dance fault in the east. The fourth block is between the Ghost Dance and the Dune Wash Faults. The fifth block is between the Dune Wash and Bow Ridge faults.

The mesh generator was run five times, once for each block, to create sub-meshes of the grid. These sub-meshes were finally combined to provide the three-dimensional grid data (volumes, connections, interfaces) for the combined grid.

The challenge in creating grid blocks located along the fault traces was to maintain the sudden offset across the faults and the correct interface to adjacent blocks. This was achieved by dividing each fault-block element in two and adapted the mesh generator in order to connect them by their common interfaces to the adjacent grid blocks (Chapter 4 in Bodvarsson et al. 1997).

2.4.3.8.4 The Combined Three-Dimensional Grid

Various programs were written to choose, check, and recombine the files with connections and volumes from these two mesh generations, as well as to allocate material properties to each model element (Chapter 4 in Bodvarsson et al. 1997). For example, one of the programs read all connection names within the output files and corrected them if they were not consistent with grid-block names. Another program combined grid blocks and their connections from different output files of the mesh generator. This program was used to add top and bottom layers of grid blocks over the entire model area to provide required boundary conditions such as saturation, temperature and pressure, during numerical simulations.

The final three-dimensional numerical grid is composed of two files, "eleme" and "conne," which contain grid-block location, volumes, and connection information suitable for a TOUGH2 input. The UZ model three-dimensional grid consists of about 39,000 primary elements and 130,000 connections (more elements and connections are required for the DKM simulation used in TSPA-VA to account for both fracture and matrix elements). The model extends vertically to the water table at about 730 m. The hydrogeological layers and the vertical offsets at all the major faults were explicitly developed by LBNL's grid-generation process. The final model three-dimensional grid shows good agreement with the geological model of Yucca Mountain (Zelinski and Clayton 1996) and is consistent with the USGS geological-framework model representation of model stratigraphy within the repository area. However, it shows significant differences in the northern and eastern part of the model. Figure 2-49 shows a plan view of the three-dimensional site-scale UZ-flow-model domain, grid, incorporated faults, and locations of boreholes. Figure 2-50 shows an east-west vertical cross-section of the stratigraphy and faults along SD-7 (B-B' in Figure 2-49).

2.4.3.8.5 Material Properties and Treatment of Layer Pinchout

Each layer was assigned material properties defined by the respective hydrogeological unit. This scheme resulted in constant layer properties for each model layer, except where pinchout or alteration of the layer occurs. When pinchout occurred, layer continuity was preserved by subtracting 3 m from adjacent layers and adding 3 m to the pinchout layers in order to preserve continuity across model layers. The pinchout was then modeled by changing material properties for the pinchout layers to those of the adjacent layers from which the pinch-out was subtracted. This material-property change scheme was used to model the pinch-out of the entire PTn2 and PTn4 layers. It was also used to model transition from the zeolitic to vitric layers in Calico Hills layers chn1, chn2, chn3 and chn4. Figure 2-51 shows the boundary maps that define the material transition in the pinch-out layers and the vitric/zeolitic interface for the LBNL 1997 three-dimensional grid.

2.4.3.8.6 Recommendations for Future Work

There is a need to harmonize the differences between the grids based on the USGS geological-framework model and the LBNL geological model in order to select a single geological model for designing future numerical grids. Work is currently underway to integrate the ISM 3.0 geological-framework model into the LBNL site-scale UZ-flow model. Integration of the ISM 3.0 geological-framework model with the site-scale UZ-flow model will increase the defensibility of the UZ modeling effort.

2.4.3.9 Summary of Implementation of the Base-Case UZ-Flow Model in TSPA-VA

The previous sections have detailed the development of the UZ-flow model used in TSPA-VA calculations. Sensitivity analyses have been performed to provide bases for parameters and conceptual models used in the three-dimensional LBNL UZ-flow model. A base case has been defined, as outlined in Section 2.4.3.1.4, and associated parameters are given in Table 2-19 through Table 2-24. The present-day infiltration used in the base case was based on the spatial-infiltration distribution described in Flint et al. (1996) (see Figure 2-18). The infiltration values were divided by 3 and multiplied by 3 to yield three present-day infiltration scenarios. In addition, these present-day infiltration scenarios were combined with variations of the fracture air-entry parameter to yield five base-case parameter sets as described in Section 2.4.3.1.4. For each, two future-climate scenarios were considered by using LTA and infiltration maps. Figure 2-19 and Figure 2-20 show the LTA and superpluvial maps for the mean present-day infiltration. These were either divided by 3 or multiplied by 3 to correspond to the value used in the present-day infiltration scenario. The resulting 15 base-case UZ-flow simulations are summarized in Table 2-37 and in the tree-diagram in Figure 2-52. For all UZ groundwater flow simulations, the EOS9 module of TOUGH2 has been used. This module implements Richards' equation and assumes that the gas phase is passive.

Once the flow fields have reached steady state, as indicated by a global mass balance within 1% error, the flow fields are used for mountain-scale transport calculations and near-field seepage studies. All developed data that are fed to other TSPA components are submitted to the Technical Data Base. These components are integrated for TSPA-VA calculations using the QA code RIP.

Section 2.5.1 presents results from the base-case simulations. Discussions of these results and their implications on performance are also presented in that section.

2.4.4 Seepage

Abstraction for seepage is based on a process model of flow in a three-dimensional block of unsaturated, heterogeneous, fractured medium to calculate the amount of water that would seep into a cylindrical opening representing the drift. A distribution of percolation rates at the repository level are calculated from the UZ model. The percolation rates are then imposed on the three-dimensional heterogeneous block for seepage calculations. Seepage calculations were made for a range of hydraulic parameters, a number of realizations, and a series of percolation rates corresponding to various scenarios studied with the UZ model. From these results, extension to other values can be made by interpolation and extrapolation of statistical descriptors.

It has been found from these studies that there is a need to include heterogeneities in the system. If a homogeneous equivalence of the medium had been used for seepage calculation, the results would have been as much as two orders of magnitude too optimistic. Seepage is found to depend on flow channeling along preferred flow paths and local ponding near the drift wall, both of which are intrinsically results of the heterogeneous field. The heterogeneous properties are taken from ESF data, where possible.

Below is a discussion of data used for input to the seepage conceptual model is given. The calculational model spans between the DKM, which represents the fractures and the matrix as two interacting continua, and the fracture-only model. Thermal-mechanical alterations, backfill, and drift collapse have not been considered. Results of the behavior of seepage under various conditions are described in Sections 2.4.4.5 to 2.4.4.10. Results show that, for steady-state conditions, the matrix does not play a strong role, and the fracture-only model is used. The steady-state data are used in the statistical results for TSPA, which are presented in Sections 2.5.2.1 to 2.5.2.4; Section 2.6.2; and Section 2.7.4.

The numerical model used in the seepage calculations, as for the site-scale model, was TOUGH2 (Pruess 1987, pp. 1-11; 1991, pp. 18-20). In following subsections, details of the model assumptions and their basis are given.

2.4.4.1 Matrix Hydrologic Properties

To simulate seepage into the drift from the heterogeneous fractured rock surrounding it, a number of property parameters are needed. Most of these are estimated based on laboratory or field measurements. This model uses properties representative of the Topopah Spring Middle NonLithophysal unit (tptpmn) at Yucca Mountain.

The matrix-porosity value of 8.9% represents the mean of all borehole measurements for the tptpmn unit (Flint 1998, p. 44). The initial matrix-liquid saturation is assumed to be in the range of 0.92. This is the value given for Borehole SD-9 (Flint 1998, p. 50). This high matrix saturation is also consistent with the laboratory data from grab samples obtained directly from the Thermomechanical Alcove (Tsang et al. 1996), where values ranging from 0.805 to 0.99 are reported.

A matrix-permeability value of 4.0×10^{-18} m^2, reported in Flint (1988, p. 44) for the Topopah Spring Middle NonLithophysal unit was used for the simulations. The matrix van Genuchten parameters have been measured in three samples from UZ-16. Values as given in Flint (1998, pp. 19-54) are 6.4×10^{-7} Pa^{-1} for α ($1/\alpha$=1.5625 MPa) and 1.47 for β (i.e., m=0.32). The residual liquid saturation is 0.18.

2.4.4.2 Fracture Hydrologic Properties

2.4.4.2.1 Stochastic Fracture-Permeability Model

Data used for the generation of heterogeneous fracture-permeability fields are mainly of two types: air-permeability tests of the drift-scale test (DST) in the ESF Thermal Test Alcove 5 (Tsang and Cook 1997) and evaluation of fracture surveys in the ESF (Bodvarsson et al. 1997, Chapter 7).

A DLS performed by the USGS/Bureau of Reclamation has provided a systematic set of fracture locations, trace lengths, and orientations in the ESF. Bodvarsson et al. (1997, Chapter 7) reviewed and analyzed the data to determine the properties and distribution of fractures along the complete length of the ESF. One type of fracture data as extracted by Bodvarsson et al. (1997, Chapter 7) is exemplified in Figure 2-53, which depicts the occurrence of fractures greater than 1 m intersecting the DLS line along the ESF from station 26+00 to 27+00. The DLS line is at y=0 in the figure. The length of each fracture indicates its observed length on the ESF wall (some being the lengths of curved lines). The orientation of each fracture shown relative to the y axis in the figure is the dip angle as estimated in the field by USGS/Bureau of Reclamation. The strike is not shown in this figure.

It is noted that fracture lengths range from the lower threshold of 1 m to lengths greater than 18 m. Most have a dip angle close to 90° (i.e., vertical), while a number of the long fractures have a dip of ~45° or less. This latter datum may be a result of bias introduced in ESF observations. Bodvarsson et al. (1997, Chapter 7) also found that in the section of ESF near the Thermal Test Alcove, the mean fracture spacing for fracture lengths greater than 1 m is 0.53 m. The data suggest a fractured rock with a dense network of short fractures (approximately 1–4 m). For fracture lengths greater than 10 m, the mean fracture spacing is estimated to be 20.9 m (i.e., long fractures are typically more widely spaced).

A series of air-permeability tests was conducted in FY-97 by Tsang and Cook (1997) in the DST. Air-permeability tests mainly measure the fracture permeability, since air flows predominantly through fractures with lower capillary suction and higher permeabilities. The tests were carried out in a set of 14 boreholes of 40 m in length, collared at the wall of the observation drift of the DST. The boreholes form divergent fans from their collars on the rock face, so that the separation distances between boreholes range from 1 m to 30–40 m. Each borehole was divided by three packers into approximately 12-m-long sections, and injection tests were carried out in each packed zone. The rock block studied in the DST is approximately $40 \times 30 \times 40$ m in dimension, which is about 30 times the rock volume studied in similar tests performed in the

SHT area in FY-96. The air-injection tests in the DST give a range of fracture permeabilities, shown as a frequency distribution of log permeability in Figure 2-54. The geometric mean of permeability is 10^{-13} m^2. It is interesting to note that the range of air-permeability values is similar to those obtained in the FY-96 SHT block (i.e., from less than one millidarcy to a few darcies).

The data from the DLS and from the DST are used to generate stochastic fracture permeability fields. The permeability values measured in the injection tests serve not only as input for generating the three-dimensional permeability fields, but also as conditioning data to the generated field. This means that, at locations where measurements are made, the generated field has values that correspond exactly to the measured values. The essential points in generating the heterogeneous fields are summarized as follows:

1. The air-permeability tests performed in the DST provide a probability distribution of fracture log permeability as shown in Figure 2-54. This permeability distribution forms the starting point for the generation of the stochastic fracture-continuum model.

2. The interference air-permeability data from the DST indicate that the fractures are well-connected, in that a pressure response to air injection is obtained in most monitoring zones. This is consistent with the borehole videos, which indicate that all the boreholes are intercepted by numerous fractures. It is also consistent with the fracture-mapping study, which shows a dense population of small fractures in the section of the ESF near the Thermal Test Alcove (Bodvarsson et. al. 1997, Chapter 7). Thus, multiply intersecting fractures are expected near the DST, forming a fracture continuum.

3. Air-permeability tests in the DST did not indicate a situation where a single large fracture cuts across the entire 30-m test domain. Though all monitoring zones respond to the injection of air, the magnitude of the pressure response is typically small in monitoring zones as compared to that in the injection zone, for all cases where distances between the injection and monitoring zones are more than 1 m. The range of distances between the injection and monitoring intervals is from about one to tens of meters in the DST air-permeability tests. This is consistent with a review of fracture-mapping data (Bodvarsson et al. 1997, Chapter 7), which indicates that long fractures are rather sparse. On the other hand, in the SHT at a nearby location (Birkholzer and Tsang 1996, pp. 15-19), where the spacing between boreholes is much smaller (distance between packed-off zones less than a meter), a fracture connection between two boreholes was more likely, and was indeed encountered.

4. Fracture mapping along the ESF displays the presence of large, widely spaced fractures, which were shown to be important (Birkholzer et al. 1996, pp. 1-48) in the calculation of fast paths for episodic flow events. For that reason, they are included in the stochastically generated permeability fields to study their effects on seepage into the drift (see below).

The experimental information discussed above is insufficient to determine the correlation structure of the heterogeneous field. We decided to adopt a correlation structure using a spherical variogram with a range of 2 m for log permeability values (in m^2) less than −12.5, which seems to be reasonable from the plots of the DLS shown in Bodvarsson et al. (1997, Chapter 7). Some sensitivity studies were performed to compare the spherical and an exponential correlation structure (DTN: LB980412541195.001 and LB980412541195.002). The differences were not significant. To account for large features observed in fracture maps, a sequential indicator code is used for the generation of the three-dimensional heterogeneous field by assigning an anisotropic correlation range of 14 m in the vertical and N-S directions, and 1.4 m in the E-W direction for log permeability values greater than −12.5 (with permeability k in m^2). Such an approach allows the generation of high-permeability vertical planes in the N-S direction to represent subvertical fractures with lengths ~14 m. The stochastic generation does not ensure a uniformly high permeability value in those planes, but the variations in these planes will have a high mean value of permeability.

Similar to an earlier study (Birkholzer et al. 1996, pp. 1-48), the sequential indicator code SGSIM of the geostatistical library (Deutsch and Journel 1992, pp. 141-142, 164-167) is used to generate the stochastic fracture continuum. The measured results of air-permeability tests in the DST block are used to condition the generated field. Note that the sequential indicator method does not require a parametric representation of the probability distribution. It directly uses the histogram of the distribution shown in Figure 2-54. Furthermore, the capability of assigning different isotropic or anisotropic correlation ranges to different segments of the permeability distribution makes it a particularly suitable tool for our purposes.

A number of three-dimensional stochastic continuum fields were generated, and sensitivity to input parameters was studied. Each of these fields has been conditioned to measured results of the DST air permeability tests. The primary case, used for most model simulations, is shown in Figure 2-55, which displays a few arbitrarily chosen planes in the generated three-dimensional block. The block dimensions are 50 m along the N-S direction (designated as the x-axis), 35 m along the E-W direction (designated as the y-axis), and 43 m in the vertical direction (designated as the z-axis). The generated field has grid blocks that are 0.5 m cubed. Note the high permeability "streaks" in the vertical and N-S directions in Figure 2-55. These represent the long, high-permeability fractures within the framework of the stochastic fracture-continuum model.

2.4.4.2.2 Other Fracture Properties

Fracture porosity and frequency are estimated by Bodvarsson et al. (1997, Chapter 7) to be 1.24×10^{-4} and 1.88 fractures per meter, respectively, based on ESF fracture mapping. No measurements exist for the fracture van Genuchten parameters. In our primary model the air-entry value is assumed to be 1,028 Pa (α=0.97 × 10^{-3} Pa^{-1}), as derived in Bodvarsson et al. (1997, Chapter 7) from fracture-aperture estimates. The van Genuchten β is chosen to be 2.7, i.e., m=0.633, as was also estimated in Bodvarsson et al. (1997, Chapter 7) based on numerically generated water-potential-versus-saturation curves for given fracture-aperture distributions. This is consistent with values calculated by Kwicklis and Healey (1993, pp. 4091-4102) and estimated in TSPA-1993 (Wilson et al. 1994, Chapter 21, pp. 1-30).

Heterogeneity is considered only for the fracture permeabilities. The other fracture and matrix properties are assumed to be uniformly distributed within the model area. We believe that the inclusion of heterogeneity in the properties of the matrix would be of minor importance, as matrix imbibition is a very slow process. However, the question arises whether the fracture van Genuchten parameters or the fracture porosity should be treated as stochastic variables. In particular, the van Genuchten α parameter is often (weakly) correlated to the permeability, and such a correlation may have a strong impact on the flow results. In soils, large permeabilities are typically related to large pore volumes, which, according to capillary theory, are associated with smaller capillary suction. In fracture continua, on the other hand, a change in permeability could be related to a change in fracture aperture or to a change in fracture density. In the first case, permeability would be correlated to the van Genuchten α parameter; in the second case, it would not. The base-case assumption for this study is the latter, uniform α.

It is important to note that the analysis presented here (as well as most other studies on unsaturated flow at Yucca Mountain) is based on the assumption of a continuous flow field in the fractures and the validity of the characteristic functions. On a small spatial scale, however, the assumption of continuity may be violated, and the discrete nature of fractures may become significant. For example, a single fracture carrying liquid vertically downward might dead-end at the drift-wall boundary, and, as connectivity to other fractures might be poor in this area, the liquid might not easily bypass the drift opening. Then, the probability of seepage into the drift would depend on whether or not the gravity-driven flow in the discrete fracture could overcome the capillary barrier at the drift wall. This is mainly a function of the fracture aperture and roughness, the length of the dead-end feature, and the amount of flux diverted into that feature. There will be additional discussion of this possibility below.

2.4.4.3 Boundary Conditions

For three-dimensional simulation runs, three blocks of dimensions 20-m high, 15-m wide and 16.5-m long are cut from the three-dimensional heterogeneous fracture-continuum field presented in Figure 2-55. The drift is represented by a horizontal open cylinder of diameter 5 m at the center of the lower part of the block (Figure 2-56). Simulation grid cells are defined to be $0.5 \times 0.5 \times 0.5$ m in order to allow efficient computation and graphing within a reasonable time frame. The three three-dimensional blocks, which we call Part 1, Part 2, and Part 3, are consecutive sections along the direction of the axis of the drift, and there is a 1.5-m overlap between the successive blocks to smooth out the differences resulting from numerical boundary effects. Thus, results are obtained and presented along a 46.5-m length along the drift.

For simulation of flow in each of these three blocks, the four side boundaries are assumed to be closed, the bottom boundary has a free-drainage (constant liquid saturation) condition, and a constant inflow is imposed on the top boundary. The inflow at the upper boundary is simulated by assigning an influx rate in a layer of boundary elements connected to both the fracture and matrix continua. These boundary elements, while having small volumes, are assigned very large interface areas with each other, so that the flux introduced in these elements is free to flow into the system according to the local effective permeabilities. Similarly, very large effective interface areas are also specified between neighboring fracture and matrix boundary elements, so that flux is free to partition between them according to their local hydraulic conditions.

The drift is assumed to be closed and sealed, and the emplaced waste is assumed to have cooled off. Thus, no thermal effects on the flow field are considered here (other projects are currently ongoing to study the thermohydrological flow processes, e.g., Birkholzer and Tsang 1996, 1997 (pp. 1-22); Nitao 1997a, pp. 1-8). After a period of time, the closed and sealed drift will have a relative humidity of 100%, the condition for a system in equilibrium. Then, the opening representing the drift acts as a capillary barrier, with zero capillary-suction pressure. This is the condition imposed at the inner model boundary for all times. The present models neglect the presence of a concrete liner at the drift walls, so that the zero-capillary-suction boundary coincides with the drift-wall boundary.

For the initial state before the introduction of a liquid pulse, a flow equilibrium between the matrix and fracture continua is simulated. Therefore, the initial fracture-liquid saturation in the model domain is directly related to the matrix initial-saturation distribution, using the van Genuchten relationships and parameters for matrix and fractures. For matrix saturation in the range of 0.92, the fracture initial saturation is essentially equal to the residual saturation (i.e., there is no flow in the fractures). The initial matrix saturation of 0.92 is achieved by applying a low percolation rate of 0.15 mm/yr, allowing the system to come to a steady state at this percolation rate, and then applying the higher percolation rate of interest, q.

Since the capillary suction in the matrix is much stronger than the capillary suction in the fractures, local equilibrium implies that the liquid saturation in the fractures will remain near zero until the matrix saturation approaches values close to 100%. Therefore, under steady-state conditions, liquid flow in fractures will become significant only for matrix saturation close to 100%.

2.4.4.4 Fracture-Matrix Interaction

Dual-permeability models require additional parameters: the interface area between fractures and matrix, and the size and shape of the matrix blocks. Both parameters are derived from the fracture-frequency value of 1.88 fractures per meter for the tptpmn geologic layer (Bodvarsson et al. 1997, Chapter 7). As with the site-scale flow model, the model can include a fracture/matrix area-reduction factor, X_{fm}, to simulate effects of reduced fracture/matrix coupling. There has been much discussion within the project about appropriate models to estimate the effective flow interface between fracture and matrix continua. Some recently proposed interface models are (1) scaling the interface area by a constant factor smaller than one, (2) scaling by liquid saturation, and (3) scaling by relative permeability (Bodvarsson et al. 1997, Chapter 7; Ho 1997, pp. 401-405; Section 2.4.2.2 of this report). Application of such interface scaling reduces the potential for mass exchange between fractures and matrix, and thereby enhances the possibility of fast fracture flow.

For the base-case model simulations, X_{fm} is set to the extreme value of zero; in fact, the matrix continuum is neglected entirely and the simulations are run with only a fracture continuum. A fracture-only model is useful if one is merely interested in the steady-state situation of percolation events. At steady state, there is equilibrium between fractures and matrix, and since matrix permeability is so low, flux occurs predominantly in the fractures for all percolation events of, say, 1 mm/yr or more. Therefore, the matrix continuum can be neglected by assigning

X_{fm}=0. However, the presence of rock matrix is important for studying the transient behavior of episodic events because water can leave the fracture continuum and imbibe into the rock matrix, making a significant difference in liquid-flow velocity down the fracture. The seepage model for TSPA-VA is based on steady-state flow results, so X_{fm}=0 should be a reasonable approximation.

2.4.4.5 Flow as a Function of Time

2.4.4.5.1 Two-Dimensional Simulations

We begin with some analyses that were done in two dimensions rather than three dimensions because of the large reduction in time for the computer runs. For these analyses, three vertical cross-sections or slices were extracted from the three-dimensional heterogeneous fracture field (Figure 2-55). The orientation of these slices is along the E-W direction; thus, the correlation length is 14 m in the vertical and 1.4 m in the horizontal direction. Each of these slices has dimension 15×20 m with a drift of 5-m diameter placed at the center of the lower 15×15 m of the flow domain (Figure 2-57). The three slices are chosen out of a random selection of the three-dimensional stochastic fracture permeability field. They appear to be different from each other visually. The three slices are shown in Figure 2-58a through Figure 2-58c. Shown is the heterogeneous permeability of the fracture continuum. Recall that the matrix continuum is homogeneous. The fracture permeability in each of these slices varies over four or five orders of magnitude. Slice 3 appears to have more uniform permeability values around the drift, while Slices 1 and 2 appear to have a stronger spatial variation around it. Slice 1 is used for most of the two-dimensional simulations.

In the two-dimensional flow simulations, each gridblock of the heterogeneous field (0.5 m $\times$ 0.5 m) is refined to 4 simulation grid blocks (0.25 m $\times$ 0.25 m) for better flow description. The initial conditions, boundary conditions, and hydrologic properties are the same as described previously.

We present results in terms of integrated flow over the upper boundary (Q_{Top}) and over the lower boundary (Q_{Bottom}). Q_{Top} is constant and corresponds to the percolation flux q; however, Q_{Top} is given as mass-of-water per time entering the model area, while q is a flux given as volume-of-water per time per unit area. Q_{Bottom} is the initial steady-state percolation rate at early times and then reaches a higher steady-state value at later times. If there is no water seepage into the drift, Q_{Top}=Q_{Bottom} at steady state. We also integrate the water flow into the drift (Q_D) as well as the water transferred between the fracture and matrix media (Q_{FM}).

The four quantities, Q_{Top}, Q_{Bottom}, Q_D, and Q_{FM} are plotted as a function of time in Figure 2-59a–Figure 2-59c for q=50 mm/yr into Slice 1 and X_{fm}=1, 0.1, and 0, respectively. Figure 2-60a–Figure 2-60c show the same results for q=200 mm/yr. The values of Q_D and Q_{FM} are plotted as negative quantities in Figure 2-59 and Figure 2-60 in order to separate the curves better. For larger q, the time at which seepage occurs is much earlier. Studying the results as a function of X_{fm}, one notes that for X_{fm}=0, when all flow occurs in the fracture continuum, seepage occurs at a very early time, and steady state is reached soon after seepage occurs. At this time Q_{Top}=Q_D + Q_{Bottom} (all Q's treated as positive). In contrast, for cases where matrix imbibition is considered (X_{fm}= 1 and 0.1), there is a slow water transfer from fractures to matrix, and the time period needed to reach steady state is much longer. In fact, the time periods shown in Figure 2-59a, Figure 2-59b, Figure 2-60a, and Figure 2-60b are not long enough to reach a steady state, as Q_{Bottom}, Q_{D}, and Q_{FM} are still changing with time. The transfer of water between fractures and matrix is large at an early time, and then slowly decreases in magnitude when the matrix becomes more saturated. The seepage into the drift, Q_{D}, occurs later than in the X_{fm}=0 case, and grows in magnitude very gently over time. Eventually, if a much longer time period with constant Q_{D} were simulated, fractures and matrix would equilibrate (Q_{FM}=0), and Q_{D} would reach an asymptotic value identical to the fracture-only case. In the X_{fm}=0.1 case, seepage occurs earlier than in the X_{fm}=1 case. However, as the matrix-imbibition rate is smaller for X_{fm}=0.1, the time to reach steady state is much larger, and the increase of Q_{D} with time is slower than for X_{fm}=1.

Figure 2-61a–d show the saturation contours in Slice 1 for q=50 mm/yr and X_{fm}=1 at four different times: (a) early time, (b) intermediate time, (c) the time when water begins to seep into the drift, and (d) a large time value. A similar set of four different times for q=200 mm/yr and X_{fm}=1 is shown in Figure 2-62a–d. Seepage into the drift occurs when the saturation of a grid element next to the drift boundary reaches 1 (i.e., it is fully saturated and its capillary suction drops to zero). This happens at different times, t_D, for different q and different heterogeneity conditions. From the progression in Figure 2-61 or Figure 2-62, one sees "fingered" or channeled flow from the top influx boundary over the 10 m towards the drift. The channeled flow is tortuous, and at several locations it may accumulate to high saturation values, dependent on the local permeability contrast. At some of these locations, the saturation may reach unity, representing a ponding condition. In principle, during a large episodic pulse, ponding is to be expected because of the heterogeneity of the system at locations where the downward flow is retarded by low-permeability grid elements below it. The drift acts as a capillary barrier, diverting flow around it. If the flow encounters a low-permeability grid element near the drift wall, water may accumulate (leading to local ponding), causing the capillary suction there to become zero, and flow will begin to seep into the drift. This is the condition for $t=t_D$. For the 50-mm/yr case, t_D is 534 days; for the 200-mm/yr case, t_D is 21 days (for X_{fm}=1).

One may remark here that this kind of ponding near the drift, and thus seepage into it, is mainly a result of the heterogeneity of the system, with its channelized flow, and the possibly large permeability contrast between neighboring rock volumes. Thus, for a homogeneous flow system, seepage into the drift is expected to occur much later, and for much higher q values. This will be shown later.

The inclusion of the matrix in a DKM provides a way for water to be transferred from the fracture to the matrix, thus significantly slowing fracture flow during the early time period. Figure 2-63a and Figure 2-63b show the saturation profiles in the matrix continuum at $t=t_D$ for q=50 mm/yr and 200 mm/yr, respectively. The figures correspond to X_{fm}=1 (i.e., full communication between the fracture and matrix continua). Note that in both percolation cases, the matrix saturation close to the location of seepage has almost built up to 1, and it can be concluded that for X_{fm}=1, seepage is possible only when imbibition into the matrix is reduced sufficiently. However, there are obvious differences between Figure 2-63a and Figure 2-63b. For 50-mm/yr percolation, seepage occurs much later, and the matrix saturations have significantly increased in the entire flow domain, while for high q, the saturation buildup to 1 is a far more localized phenomenon. If X_{fm}=0.1, there is a 90% reduction of the exchange between fractures and matrix, and the matrix saturation increase is drastically reduced because the imbibition rate is smaller, as shown in Figure 2-64a for q=50mm/yr (compare to Figure 2-63a). In this case, flow in fractures is stronger and the time for seepage into the drift is shorter (t_D=8.4 days). Saturation contours in the fracture continuum at t_D are shown in Figure 2-64b. The saturation results for the limiting case of X_{fm}=0, where flow is essentially restricted within the fracture (fracture-only case), are presented in Figure 2-64c. Here, in the absence of matrix imbibition, seepage occurs after only t_D=2.1 days.

Based on the above calculations, the seepage initiation time t_D can be studied as a function of q. This is presented in Figure 2-65 for the X_{fm}=1, X_{fm}=0.1, and X_{fm}=0 (fracture-only) cases with percolation rates of 25, 50, 100, 200, 500, and 1,000 mm/yr. A percolation of q=5mm/yr was also modeled, but had no seepage for any of the X_{fm} models; therefore, this case is not shown in the figure. The 5-mm/yr run represents the current estimate of steady-state percolation flux at Yucca Mountain (CRWMS M&O 1998. *Yucca Mountain Site Description*, Section 5.3.4.1).

Figure 2-65 shows that, as q becomes smaller, t_D increases dramatically. In cases of very large t_D one must keep in mind that seepage will be observed only if the respective percolation rate is sustained at least up to t_D. Therefore, the probability of seepage depends, among other factors, on the flow-event duration. Studying the results as a function of X_{fm}, one notes that the seepage initiation time for X_{fm}=1 is much larger than for X_{fm}=0. The X_{fm}=0.1 results are close to the X_{fm}=0 results at larger percolation flux, but close to the X_{fm}=1 result at low-flux values. This shows that the effect of different X_{fm} values depends on the percolation event, as the pulse size affects the pulse-propagation velocity and thus the time period during which the flow exchange occurs between fractures and matrix.

Figure 2-66 presents the rate of seepage as a function of the percolation rate, calculated at large times when a steady state is reached. The steady-state seepage rate into the drift is expressed as a fraction of the inflow into the model area over a 5-m width of the upper boundary (i.e., over the width [or diameter] of the drift). Only the X_{fm}=0 results are used for this calculation, as the fracture-only cases run to steady state in much shorter time periods. Note from Figure 2-66 that the relative seepage rate steadily increases with the percolation rate, from 10.2% at 25 mm/yr to 93.6% at 1,000 mm/yr for Slice 1. In other words, the absolute amount of seepage flux into the drift at 1,000 mm/yr would be about 360 times larger than that at 25 mm/yr. At 1,000 mm/yr, a seepage rate of 93.6% indicates that only a minor fraction of the percolation flux is diverted around the drift. The drastic increase in drift seepage flux with percolation rate demonstrates the importance of a good estimate of the percolation flow rate.

Figure 2-67 shows the seepage-initiation times for Slices 2 and 3, together with the Slice-1 results for comparison. The time when water first seeps into the drift is larger for Slice 3 (and even larger still for Slice 2) in all cases considered. It is interesting to note that for Slice 2, seepage occurs only at percolation rates of 500 mm/yr or more. For lower fluxes, flow is able to find a path around the drift. For Slice 3, water seeps into the drift for 50-mm/yr percolation or more. These results are not obvious from a superficial study of the permeability fields in Figure 2-58a through Figure 2-58c. There, it appears that Slice 2 is similar to Slice 1 (in a statistical sense), but Slice 3 has a relatively homogeneous region around the drift. However, a closer examination of these figures shows that there is a local blockage on the right side of the drift in Slice 3 that causes water to accumulate there and enter the drift. On the other hand, for Slice 2, water is able to flow around the drift in most percolation cases (except for those with very large percolation rates). This raises two interesting points. First, seepage into the drift versus flow around it depends on details of the heterogeneity in the vicinity of the drift; since it is not possible to know all the details, a stochastic approach is needed. The differences in results for the three slices give a feeling of the dependence of results on alternative realizations. And second, a high-permeability "skin" around the drift (as a result of construction or other reasons) may act to enhance diversion of flow around the drift; this deserves further investigation.

Figure 2-68 gives the steady-state relative seepage rates obtained for Slices 2 and 3 compared to Slice 1, indicating that in all cases seepage for Slices 2 and 3 is significantly smaller than for Slice 1.

As a comparison to the above cases, in which the fracture continuum is heterogeneous, calculations were made by assigning a constant fracture permeability of 10^{-13} m^2 for the entire fracture continuum. Furthermore, it was assumed that X_{fm} is equal to zero (fracture-only), which is the case where t_D is the shortest. For q=200 mm/yr and X_{fm}=0, t_D is found to be less than 1 day (see Figure 2-65) in the heterogeneous case.

The saturation contours for the homogeneous case with X_{fm}=0 and q=200 mm/yr are shown for three times in Figure 2-69a–c. At the longest time shown (900 days), the flow has attained steady state. It is noted that no seepage into the drift occurs; water flows downwards around the drift on both sides. This shows clearly that the early seepage found above is mainly a result of heterogeneity and channelized flow in the fracture continuum. This is confirmed by the work of Nitao (1997b, pp. 1-8), who also performed a modeling study of flow around a drift and found that homogeneous models under-predict the seepage that can occur, because they do not account for the preferential flow paths that begin to "weep" at low fluxes. One also notes in Figure 2-69 that saturation builds up at the crown and upper sides of the drift, reaching values of 0.45 to 0.75 from an initial value of less than 0.05. This increase of saturation results in a significant increase in effective permeability near the top part of the drift, thus promoting an increase of flow around the drift so that no seepage occurs.

2.4.4.5.2 Effects of Episodic Pulses

In this section results of a study considering effects of a series of episodic percolation pulses are presented. Nitao (1997c, pp. 1-13) has also analyzed seepage resulting from episodic percolation.

To study effects related to the periodicity of episodic flow events, the case with q=50 mm/yr and X_{fm}=1 is considered. Let q last for a time period t_p and then let its value drop to a constant level of 0.15 mm/yr for an interval of t_i. Then at $t=t_p + t_i$, q is set again to be 50 mm/yr for another period of t_p. A schematic diagram is shown in Figure 2-70. For modeling, the case where t_p=1 year and t_i=9 years is considered.

First, in Figure 2-71a, fracture-saturation contours at the end of a single pulse of 1-year duration are presented. After 1 year, q is reduced to 0.15 mm/yr. Figure 2-71b and Figure 2-71c shows the saturation contours at t=10 years and t=1,000 years, respectively, without any subsequent pulses. (Note the different scales for the saturation contours in Figure 2-71a and Figure 2-71b through c.) No seepage into the drift occurs in this case. It is seen that at t=10 years, the fracture saturations have dropped significantly compared to the situation immediately after the single pulse event, but they are still significantly higher than the initial saturation of about 1%. The saturation after 1,000 years is similar to the 10-year situation, indicating that the system has still not recovered from the large pulse. Apparently, some portion of the water accumulated during the 1-year pulse is still being held in the matrix pores, and is very slowly draining into the fractures. Therefore, consecutive pulses as described above, with t_p=1 year and t_i=9 years, will certainly show interference and cannot be considered as independent. However, this effect is expected to be less significant in the case of X_{fm}=0.1, or in other reduced-interface cases.

From the above results, it may concluded that a second pulse of 1-year duration, starting after an interval period of t_i=9 years, will have a very different flow condition (at t=10 years) than the first pulse starting at t=0, as the saturation (and the relative permeability) is higher along certain flow paths, thus allowing for faster flow through the system. This effect would be even stronger for a third pulse, starting 9 years after the second pulse; and a fourth, starting 9 years after the third, etc. In Figure 2-72a–Figure 2-72b, saturation contours at the end of a second pulse and at the end of a third pulse are presented, respectively (compare with Figure 2-71a for the first pulse). Seepage into the drift occurs (at some point in time) during the second pulse. Continuing the simulation for the third cycle, one finds that the seepage occurs right from the beginning of the third pulse. The results are summarized in Figure 2-72c, where Q_D is shown as a dotted curve together with Q_{Top}, Q_{Bottom} and Q_{FM} for all the three cycles. As a result, successive pulses can result in drift seepage in cases when seepage would not occur for a single, independent flow event.

2.4.4.5.3 Three-Dimensional Simulations

Figure 2-73 shows the fracture-permeability distribution on three arbitrarily chosen vertical planes of the three-dimensional block, Part 1. The permeability variation ranges over three orders of magnitude consistent with the input data (see Figure 2-54). The saturation profile on the same planes after 1 day of 1,000-mm/yr percolation is shown in Figure 2-74 for X_{fm}=1. It is obvious that gravity-driven flow occurs along the high-permeability areas, with lateral diversion because of low-permeability parts. While the liquid front is moving in the fracture continuum, there is imbibition into the matrix continuum that is not shown here.

Saturation profiles on horizontal planes for the same case are shown in Figure 2-75a through d. For a plane near the top (Figure 2-75a), the gravity flow is distributed among high-permeability locations. This focusing or channeling of flow in a few locations appears to persist at lower levels (Figure 2-75b). Figure 2-75c shows the saturation profiles on the horizontal plane just above the drift. Here the capillary-barrier effect introduced by the drift comes into play; the vertical flow slows down and liquid accumulates at the crown of the drift. This accumulation of liquid is very significant in some areas where the flow diversion around the drift is blocked by nearby low-permeability areas. In these areas, the saturation may build up close to 1, the local capillary suction decreases close to zero, and seepage into the drift can occur. Figure 2-75d shows the saturation profile on a plane below the drift. One notes the low-saturation shadow of the drift, as well as the higher-saturation areas on the right-hand side. The latter is the result of the flow bypassing the drift on its way downwards under gravity.

As in the two-dimensional cases, all the inflows over the upper and the outflows over the lower boundary are integrated as Q_{Top} and Q_{Bottom}, respectively. The total inflow Q_{Top} is constant in time, while Q_{Bottom} is zero at early times and then reaches a steady-state value at later times. The two values must be equal at steady state if there is no seepage into the drift. The total seepage rate into the drift Q_D and the water transfer from the fracture to the matrix continuum Q_{FM} are also calculated. These four quantities, Q_{Top}, Q_{Bottom}, Q_D, and Q_{FM} for the three-dimensional block Part 3 are plotted as a function of time in Figure 2-76a and Figure 2-76b for the full-connection case (X_{fm}=1) with q=200 mm/yr and 1000 mm/yr, respectively. The corresponding results for X_{fm}=0 (fracture-only) are shown in Figure 2-77a and Figure 2-77b. In general, Q_D is zero at early times because the pulse has not yet arrived at the drift. At a time indicated by a circle in the figures, seepage occurs and Q_D becomes nonzero, though usually at a small value compared with the percolation rate Q_{Top}. Naturally, the seepage initiation time is much later for X_{fm}=1 than X_{fm}=0, due to the retarding effect of matrix imbibition.

Based on the above and similar calculations, the seepage-initiation time, t_D, as a function of the percolation flux is studied. Results are presented in Figure 2-78 for X_{fm}=1 and 0. Seepage occurs for Parts 1 and 2 at percolation rates of 25 mm/yr and higher; for Part 3, seepage is obtained only at 100 mm/yr and higher. (Remember that the simulation period in some of the X_{fm}=1 cases is not long enough to allow for seepage to occur.) Comparison with the two-dimensional results indicates that the behavior is qualitatively similar. The percolation threshold of seepage into drifts is in the same range for the three-dimensional and the two-dimensional runs. Also, the seepage-initiation time is in the same range for two-dimensional and three-dimensional results. A possible reason is that since seepage is related to channeled or focused flow, there is qualitatively little difference between one-dimensional (tortuous) channels in two-dimensional or three-dimensional space.

Figure 2-79 shows the rate of seepage as a function of the percolation rate for X_{fm}=0. The rate of seepage is expressed as a fraction of the percolation flux over an area corresponding to the area of the drift projected onto the upper inflow boundary. Note that, as a result of computational limitations, some of the runs for Part 1 (100, 200, and 500 mm/yr) did not reach steady state, and are thus not included in the figure. The relative seepage rates range from very small values at 25 mm/yr to about 30% at 1,000 mm/yr. These values are consistently smaller than in the two-dimensional simulations, a possible result of flow bypassing local ponding conditions in the third dimension.

The three rock blocks considered in this study show significant variation among them, which appears to be in a similar range as the variation among the two-dimensional slices. This indicates the need for a stochastic approach for deriving the probability, the spatial distribution, and the rate of seepage into drifts.

The spatial distribution of seepage is also important, as it determines how many waste packages could be affected by the seepage. The seepage distribution is dependent on the heterogeneous field and various parameters used in our model, such as the permeability-probability distribution, spatial-correlation lengths, and values of van Genuchten parameters. The calculated seepage pattern is shown in Figure 2-80 and Figure 2-81 as saturation contour plots on the drift wall. The drift wall is represented by a plane, with one axis corresponding to the drift axis and the other axis corresponding to the curved distance from the crown of the drift to the bottom. Since the drift is 5 m in diameter, the curved distance ranges from $-5\pi/2$ to $+5\pi/2$ m.

In these figures, a montage is formed from all three three-dimensional blocks, Parts 1, 2, and 3 (see Figure 2-56), so that the total drift length along the x-axis is 46.5 m. The areas with saturation above 0.999 are shaded, and indicate locations where seepage is likely to occur. Figure 2-80 shows results for the full-connection model, X_{fm}=1, and 1,000 mm/yr. Figure 2-81 shows the corresponding fracture-only case, X_{fm}=0. A distribution of seepage locations and saturation contours are seen, with the seepage more likely to occur around the crown of the drift, as one would expect. While the size of the seepage areas is larger for the fracture-only case, the locations of the seepage areas (represented by the centroid of each area) will be similar to that of the full-connection model at large times. From these results, with this particular set of parameters, the spacing between the seepage areas is of the order of about 15 m. This may be related to the anisotropic spatial correlation used in generating our heterogeneous field, which assumed a correlation length for large-permeability values of 14 m in the vertical and N-S direction and 1.4 m in the E-W direction (see Section 2.4.3.2.1).

2.4.4.6 Sensitivity to Fracture-Hydrologic Properties

This section describes results of a sensitivity study for the fracture van Genuchten parameters α and β. Three different parameter variations are considered: (1) a change in the value of β, (2) a change in the value of α, and (3) a change in the conceptual model, allowing α to correlate with the local permeability. In all three cases, all other parameters are kept the same as the primary parameter set. In the first case, the original value of β=2.7 is changed in the primary parameter set to β=1.97, and Slice 1 for X_{fm}=1 and X_{fm}=0 is considered. This new β value is chosen from calibration results from the UZ site-scale model (Bodvarsson et al. 1997, Chapter 6). A similar calculation is performed for the second case using $\alpha=2 \times 10^{-4}$ Pa^{-1} instead of the original value of $\alpha=9.73 \times 10^{-4}$ Pa^{-1}. The two cases with different van Genuchten properties are chosen so that seepage into a drift is expected to be less likely compared to the primary parameter set, because the new parameters give rise to stronger capillary suction in the flow domain for a given percolation rate. Note, for example, that for a free-drainage flow of 50 mm/yr in a homogeneous fracture domain, capillary suction and saturation are -2,453 Pa and 22.3%, respectively, for the primary parameters, –3,139 Pa and 32.9%, respectively, for β=1.97, and –11,930 Pa and 22.3%, respectively, for $\alpha=2 \times 10^{-4}$ Pa^{-1}.

For the case with permeability-correlated α, the following scaling relation is assumed between the local α-value and the local permeability, k, after Leverett (1941, pp. 152-169):

$$\alpha = \bar{\alpha}\sqrt{\frac{\bar{k}}{k}} \quad , \tag{2-36}$$

where $\bar{\alpha}$ and $\bar{k}$ are reference values, chosen to be 9.7×10^{-4} Pa^{-1} and 10^{-13} m^2, respectively. As discussed in previous sections, the reference value for fracture permeability is the geometric mean reported by Tsang and Cook (1997) and the reference $\bar{\alpha}$-value is derived in Chapter 7 of Bodvarsson et al. (1997).

Figure 2-82 and Figure 2-83 show, for Slice 1, the seepage-initiation time and the seepage rate, respectively, as functions of the percolation rate for the new cases, and include results obtained with the primary parameter set for comparison. For the new β value, seepage is obtained for all percolation fluxes of 25 mm/yr or higher. For the new α value, seepage is found for fluxes of 50 mm/yr and higher. In the case of α being correlated with permeability, seepage occurs for flows of 100 mm/yr and higher. This correlation tends to smooth unsaturated flow in heterogeneous permeability fields. Assuming that high-permeability features are typically correlated with weak capillary suction, they tend to be conductive only at large percolation events. The initiation times and seepage rates of all cases are found to differ from those obtained with the primary parameter set by less than one order of magnitude. For the initiation times, a consistent trend is observed for all the runs with α=2 $\times$ 10^{-4} Pa^{-1}. Here, the seepage occurs later for both the X_{fm}=1 and 0 results, as the capillary suction in the fractures is stronger than in the base case. For seepage rates, all runs using the new β value give a slightly higher flux into the drift than the primary case. In contrast, cases of permeability-correlated α show seepage rates consistently smaller than the primary case. This is because, for permeability-correlated α, the flow field is smoother and tends to be closer to the homogeneous case.

An additional calculation was performed in three dimensions to confirm that changes in the van Genuchten β have little effect on seepage. For a percolation flux of 213.4 mm/yr into Part 1, β was changed from its primary value of 2.7 to a new value of 2.0. The obtained seepage rate changed minimally from 12.78% to 12.79%. Thus, for the steady-state situation, the seepage rates are not very sensitive to the value of the β parameter. However, this conclusion would change if one were interested in the transient response of the system to episodic flow events.

Additional three-dimensional results showing sensitivity to variations in fracture α and permeability are presented in the section on base-case results (Section 2.5.2). Those results confirm that the amount of seepage in the model depends sensitively on fracture α and k.

These analyses demonstrate that the seepage times and rates are controlled by several factors-including percolation rate, rock properties, and the fracture/matrix interaction in a highly nonlinear manner.

2.4.4.7 Effect of Discrete Fractures at the Drift Wall

This section examines the effect of relaxing the assumption that the fractures form a continuous flow field that allows lateral flow around the drift at any given location. The alternative conceptual model is that there may be discrete features close to the drift wall that do not have a lateral connection to the continuous fracture network. In that case, water carried in these features cannot bypass the drift. The probability of seepage may greatly increase, depending on whether or not the gravity-driven flow in the discrete fracture can overcome the capillary barrier formed by the drift wall. This phenomenon is essentially determined by aperture, roughness, spatial orientation of the fracture, length of the fracture section, and the amount of flux diverted into the fracture. A case is simulated assuming constant-length discrete features of 0.05-m vertical extension, connected to the continuous fracture network only at their upper end, and connected to the drift wall at their lower end. Otherwise, the primary-case properties and the same heterogeneous field is used as before.

The new conceptual model is simulated by adjusting the discretization of the mesh near the drift wall. All computational fracture-continuum elements adjacent to and above the drift wall are assigned a vertical connection distance of 0.05 m to the drift. Thus, over this given distance there is no connection for the flow to go laterally to circumvent the drift, and gravity-flow may lead to an accumulation of water at the drift wall. (Note that in all other model runs, the connection distance of fracture-wall elements was set to zero, thereby implicitly assuming that these elements are in the immediate neighborhood of the drift.) The permeability assigned to the discrete connections is assumed to be equal to the continuum permeability of the heterogeneous field at that particular location. It is thereby implied that all fractures close to the wall are vertical fractures without lateral connection, and that therefore the potential permeability of these discrete features is in a range similar to the permeability of the fracture continuum. This is certainly a worst-case assumption, as the mining process and the long-time alteration will induce additional fracturing close to the drift walls, thereby locally increasing the connectivity of the fracture network and decreasing the probability of nonconnected discrete features.

The simulation runs were performed using a 213.4-mm/yr percolation flux. For the run with discrete fractures of 0.05-m length, the seepage rate increased to 21.56%, which is to be compared with the original value of 12.78%. Therefore, the presence of discrete features has a potential for significantly increasing the drift seepage; however, more refinement of the conceptual model is needed, with better estimates of the likelihood of discrete features, their geometry, and their properties. Fracture-network studies based on fracture mapping might help to achieve this goal. The ongoing niche liquid-release tests should also provide a preliminary evaluation of the relative importance of discrete features along the drift walls.

2.4.4.8 Sensitivity to Mesh Resolution

All simulations aside from this subsection use a grid discretization of 0.5 m on a side (i.e., the numerical flow grid has the same resolution as the generated geostatistical permeability field). To study the sensitivity of the simulation results to the numerical grid resolution, additional simulation runs were performed, with refined grids for a two-dimensional vertical cross section perpendicular to the drift center line. The original 0.5-m × 0.5-m discretization is refined by dividing each grid block first into 4 sub-blocks and then into 9 sub-blocks. The sub-blocks have assigned the same permeability value as the original grid block (i.e., the heterogeneity structure remains unchanged). Results indicate that there is some sensitivity to the grid design, as the derived seepage rates increase when using a finer grid resolution (DTN: LB980412541195.001 and LB980412541195.002). This is mainly because the gradients between elements of different permeability are steeper in a simulation with fine sub-gridding, while a simulation with the original grid—identical resolution of heterogeneity field and simulation grid—has smoother transitions as a result of the harmonic weighting of the two neighboring permeability values at element interfaces. One must consider that the assumed step-change of permeability in the generated random fields is only an approximation of the more smooth transition in natural domains. Therefore, the original grid design may actually allow for a reasonable representation of natural heterogeneity. If the permeability values for the refined grids were derived by interpolation from the underlying random field to smooth out the strong step-changes, the impact of the mesh refinement would probably be small. More work along this line will be performed in future studies.

2.4.4.9 Comparison With ESF Niche Tests

This section presents modeling efforts to match results obtained from the liquid-release tests performed in Niche 3650 on November 14 and 15, 1997 (Wang et al. 1997). These tests were performed in the ESF under QA program; hence the results are Q-data. Liquid water was released from a horizontal borehole located roughly 0.67 m above the ceiling of Niche 3650; see Figure 2-84. The water was injected in five test intervals of 1-foot-length each; the injected mass was roughly 1 kg, with injection rates of 0.52 g/s up to 2.88 g/s. (Note that these injection rates give rise to liquid fluxes that are very high ($\sim 10^5$ to 10^6 mm/yr) compared to any of the estimated percolation fluxes of present-day or future-climate scenarios.) Before these tests, the fracture permeability in each interval was measured by air-injection tests. Injected water that reached the drift ceiling and eventually dripped into the niche was collected using a custom-designed tray constructed with 1-foot by 1-foot resolution. The total mass of water that dripped into the drift was measured, and the timing of dripping was recorded.

Table 2-38 gives some details concerning the five injection tests. It is important to note that the injection rate into the borehole in some cases (Tests 1 and 3) exceeded the saturated hydraulic conductivity of the fractured rock mass surrounding the packed-off interval. In such cases, the injected water is stored in the borehole interval, creating a ponded situation. The borehole storage capacity is limited to approximately 0.8 liters of fluid; if that volume is exceeded, water is released from the interval to prevent strong pressure buildup. This type of release actually happened in Test 5. (About 70% of the injected mass was returned; therefore, the adjusted injection rate for Test 5 is 30% of the 1.85 g/s.) In other cases (Tests 2 and 4), the injection rate into the borehole was smaller than the saturated hydraulic conductivity of the fractured rock, so the injected liquid could immediately flow into the adjacent rock mass.

A relative humidity of 100% is assumed to exist in the niche close to the walls, and the niche is assumed to act as a capillary barrier to the injected water. To understand the test results, it is very important to consider the nature of the flow field close to the borehole for the different test cases. When the injection rate is large compared to the saturated conductivity of the fractured rock, the flow condition in the borehole vicinity will be close to saturated, and seepage into the underlying niche is likely. Thus, seepage should be expected for Test 1 and Test 3. If the injection rate is smaller than the saturated conductivity, the flow field will be unsaturated, and seepage is less likely (Test 2 and Test 4). Indeed the test results in Table 2-38 show that about 22.5% to 27% of the injected water seeped into the niche for Test 1 and Test 3. Only 9.5% of the injected water was captured for Test 2, where the measured fracture permeability is about 100 times higher than in the other intervals. No seepage was observed for Tests 4 or 5. The experimental data seem to confirm our understanding of the niches acting as capillary barriers, suggesting that there is some threshold percolation flux for seepage to occur.

As a first-order calculation to test the drift-seepage calculational results against observed data, the liquid-release tests were simulated using a similar conceptual model (i.e., the niche is assumed to act as a capillary barrier for the gravity-driven liquid flow in the fractures). The injection interval in the borehole is explicitly modeled by assigning a storage capacity of 0.8 liters. In a first series of simulations for the five injection tests, a single-fracture-continuum model is employed, assuming homogeneous properties. The fracture-permeability values are estimated from the air-injection tests performed for the particular intervals tested. Fracture porosity and van Genuchten parameters are assumed to be the same as the primary-case values described previously; no parameter adjustment or calibration is performed. Note that the injection in Test 5 is simulated using only 30% of the total injection rate, because 70% of the injected water was released from the interval because the borehole storage capacity was exceeded.

Table 2-39 gives the simulated test results, presenting the seepage percentage, time of first arrival, and duration of dripping for the five tests. Overall, the agreement with the test results is very good, which is particularly remarkable when considering the relative simplicity of the model. For Tests 1 and 3, the amount and the timing of seepage into the niche are well represented by the model. In Test 2, our initial model predicts that there would be no seepage, because there is very large fracture permeability, which can effectively divert the injected liquid around the drift. However, if this large permeability is conceptualized as stemming from one distinct vertical fracture set, and if this concept is introduced in the model by assigning an anisotropic permeability structure with a two-orders-of-magnitude smaller permeability in one horizontal direction, the observed behavior can be matched quite well.

In a second step, the Test-3 configuration is used to study the effect of introducing fracture heterogeneity. The same heterogeneous permeability field is applied as in the primary seepage model (Figure 2-55), but all permeability values are scaled to arrive at a geometric mean equal to the measured air-permeability value. A spatial down-scaling by a factor of six is also performed to get a correlation length of 0.33 m, which is equal to the length of the borehole intervals. The standard deviation of permeability values around the mean is not changed in this procedure; it is identical to the one used for all the drift-seepage simulations. Using this permeability structure, the simulated seepage volume is 34.7%, compared to 19.6% simulated in the homogeneous run, and compared to 27.0% as experimentally measured.

Additional runs were performed to study the effect of matrix imbibition. (In contrast to the steady-state assumption used for the base-case seepage model, the niche liquid-release tests are transient events, and matrix imbibition might be important.) A dual-porosity model was employed, representing the matrix rock with the Multiple Interacting Continua method (MINC), using matrix properties representative for the tsw34 (tptpmn) unit at Yucca Mountain.

Simulation results for Test 3 indicate that matrix imbibition reduces the seepage volume to some extent, but does not significantly affect the liquid-pulse propagation on the small scale considered. It can therefore be concluded that an experimental observation of small or no seepage into the niche is most likely not a result of the liquid imbibing into the matrix.

The effect of a different representation of the niche-wall boundary was also investigated. In Test 3, the liquid arriving at this boundary was assumed to readily drain into the drift, without any capillary-barrier effect. In that case, 87.4% of the injected water seeped into the drift. In two other runs, the presence of vertical discrete fractures at the drift wall with no lateral connection to the fracture network, considering fractures of 0.05-m and 0.25-m length (see Section 2.4.3.7) was assumed. In the first case of 0.05-m-long discrete fractures, about 43.4% of the injected mass was captured in the niche; in the second case, it was more than 80%, which is to be compared to the measured value of 27%. Thus, the hypothesis of the niche acting as a capillary barrier appears to be valid; in particular, an assumption of free drainage at the wall or an assumption of 0.25-m-long discrete fractures leads to an overestimation of the liquid volume captured in the niche.

The conclusion of this preliminary modeling exercise is that seepage rates were obtained that correspond well to the experimental observations by using our conceptual model for the drift-seepage simulations. One must note, however, that both the niche liquid-release testing and the associated modeling efforts are still in progress.

2.4.4.10 Summary

Following is a summary of important points about the base-case seepage model.

1. Heterogeneity in the flow domain is critical for the calculation of seepage. It causes channelized flow and local ponding, so that the probability of seepage is much larger, and the time required for seepage into the drift is much shorter, than for the case where the flow domain is assumed to be homogeneous.

2. The conceptual model for the interaction between fractures and matrix (i.e., X_{fm}) is important for transient flow in the case of episodic percolation events. Field-scale studies like the niche experiment can provide information on the "effective X_{fm}" value. However, in considering long-term climate changes, the primary interest is seepage under steady-state conditions, so that fracture-matrix interaction need not be considered.

3. In general, seepage time decreases and seepage rate increases with an increase in percolation rate. The relationship between seepage and percolation is not linear, because of the many nonlinear processes involved.

4. Variation among geostatistical realizations is significant (though within the same order of magnitude) and dependent on details of local heterogeneity around the drift. Since such details are not known, a stochastic approach is necessary.

5. Comparison between two-dimensional and three-dimensional runs indicates that the probability of seepage and the seepage-initiation times are similar. The relative seepage rate, however, appears to be different in the three-dimensional runs, due to the possibility of flow in the third dimension.

6. The three-dimensional runs offer the opportunity of evaluating the possible spatial distribution of seepage along emplacement drifts, which cannot be achieved using two-dimensional vertical cross sections. The spacing of seepage locations is dependent on the correlation lengths of spatial heterogeneity.

7. For our model, seepage is insensitive to the van Genuchten β parameter of the fractures. Seepage is sensitive to fracture α and permeability (k). For steady state, seepage is not sensitive to the matrix hydrologic properties. For transient problems, and for percolation rates lower than those considered here, matrix properties may be more important.

8. There are important questions about the effects of the discrete nature of fracture flow, especially the possible role of fractures that dead-end at the drift wall. The preliminary niche-test results appear to fit the base-case conceptual model well, but more analysis (and testing) is needed.

2.5 BASE CASE ANALYSIS

2.5.1 UZ Flow

Results of the base-case UZ flow simulations summarized in Table 2-37 and in Figure 2-52 are presented in this section. The results are presented in three categories: (1) liquid saturations and perched water, (2) percolation fluxes and fracture-matrix partitioning, and (3) travel time between the repository and water table.

2.5.1.1 Liquid Saturations and Perched Water

Comparisons to liquid saturations along vertical columns were performed to verify the proper calibration of the models. The simulated matrix saturations at borehole SD-09 are shown in Figure 2-85 through Figure 2-87 along with measured data for three present-day cases: minimum fracture alpha and present-day infiltration divided by three (mnad3_p); mean fracture alpha and present-day infiltration (mnaqb_p); and maximum fracture alpha and present-day infiltration multiplied by three (mxax3_p). Similar results are shown in Figure 2-88 through Figure 2-90 for SD-12, which is further south along the repository. Comparisons are generally good, and matrix saturations tend to match observed values within the various geologic units. Good matches were also obtained between predicted and observed perched water elevations and saturations at boreholes UZ-14, SD-12, SD-9, SD-7, NRG-7a, and G-2 (Wu et al. 1998, p. 57).

Simulated perched-water bodies and their volumetric extent were examined using several two-dimensional plots that display results extracted from three-dimensional model output. Figure 2-91 is a plan view showing water saturation contours along the top of the CHn zeolitic unit, clearly indicating that an extensive perched-water body surrounds Boreholes UZ-14, SD-9, NRG-7a, and G-2 from south to north. The simulation results of Figure 2-91 are from the base-case, present-day infiltration scenario ("mnaqb_p" in Table 2-37). It is also interesting to note that relatively higher saturation values exist to the northern part of the model domain, where the higher infiltration rates are located, and in the southern part the lower saturation zone corresponds to the vitric "holes" in the CHn. The actual northern boundary of the perched zone may extend beyond the northern model boundary, as shown in the figure, based on the high infiltration rates inferred for this area. Figure 2-91 shows very low saturations along the major faults due to higher permeability and low capillary-suction forces in the fault zones. Other base-case simulations shown in Table 2-37 produced similar, extensive perched bodies surrounding UZ-14, SD-9, NRG-7a, and G-2.

Simulated vertical profiles of the perched-water bodies can be seen in Figure 2-92, where fracture-liquid saturations along two vertical cross-sections (one in the northern part of the repository at N235,000 and one to the south N233,400) are shown. An extensive water body exists in the northern part of the repository, and the simulated perched-water body location matches observed perched-water data at Borehole UZ-14. No perched water is seen in the vicinity of the repository (denoted by the white line) in the vertical cross-section to the south.

In each cross-section in Figure 2-92, unretarded tracers (no matrix diffusion, no sorption) were released at two surface locations (10 particles at each location) above the left and right ends of the repository. The open symbols denote a higher concentration of the tracer in the fracture, while the solid symbols denote a higher concentration in the matrix. In both cross-sections, flow is nearly vertical above the repository, except for some lateral movement in the matrix of the nonwelded PTn unit. In addition, the flow is contained primarily in the fractures of the welded units and in the matrix of the nonwelded units. In the north cross-section, a significant amount of lateral diversion exists below the repository because perched water is present. Tracers released along the left end of the repository traverse above the perched water for hundreds of meters to the right before entering the water table. Some of these tracer particles also partition into the matrix upon reaching the perched water and traverse laterally below the perched water. In the south cross-section, although perched water is not prevalent, some lateral diversion beneath the repository still exists. The diversion is likely caused by the contact of the Calico Hills vitric and zeolitic units, where a large disparity in matrix permeability exists.

The simulated minimum volume of perched water at UZ-14 can be estimated by examining the simulated perching areas and the perched-water thickness. As indicated in Figure 2-91, which shows the plan view of the perched water for the present-day infiltration scenario, the perching area at UZ-14 is at least 1,000 m × 1,000 m, and the perching thickness is at least 50 m according to the north cross-section in Figure 2-92. Therefore, the perched-water volume is 5×10^7 m^3. This is in agreement with the perched-zone volume estimated from analysis of pump test results (Wu et al. 1997).

Finally, calibration results to ^{14}C data (Yang et al. 1996, pp. 45-57, 55) can also be made with the base-case simulations. The C-14 data collected by the USGS provide very important information regarding (1) much "younger" water existing in the CHn unit, and (2) possible fast flow pathways from the ground surface to the CHn unit. The conceptual model used is that water flows down from the area of the Solitario Canyon Fault, and then moves laterally along some high-permeability layers in the CHn unit below the perched-water zones. The methodology for assessing this conceptual model of flow was as follows:

- Obtain the steady-state flow field corresponding to each infiltration case.
- Use the steady-state flow field to study the transport behavior of a tracer assumed to be put at the ground surface with constant concentration.
- Obtain breakthrough curves at a number of nodes in a vertical plane to ascertain the concentration vs. time data. The nodes chosen were situated near UZ-14 and were distributed so that differences in the zones at and below the perched water could be investigated.

The infiltration rate and the parameter set used correspond to the calibrated base-case, present-day infiltration scenario. The tracer was treated as a conservative component without radioactive decay, ignoring the hydrodynamic dispersion through the fracture/matrix system. The molecular diffusion coefficient in the matrix was 10×10^{-10} m^2/s.

The normalized breakthrough curves for the base-case, present-day infiltration rate of 4.9 mm/yr shows distinctly higher concentration in the zones below the perched water compared to the perched-water zones (Wu et al. 1997). In the zone below the perched water, the normalized concentration (normalized with respect to the boundary concentration) of 0.2-0.5 was reached at about 2,500–5,500 years compared to concentrations of 0.1-0.3, less in the perched-water zones for the same time period. The higher concentration below the perched water compared to the perched-water zone suggests the existence of fast pathways from the surface carrying the infiltrating water to these zones along the Solitario Canyon fault. A faster travel time would then lead to younger water (in age) below the perched layers in contrast to older waters in the perched zones. The tracer transport results for the high infiltration and the low-infiltration cases were evaluated, and found to have similar behavior. The younger water was located below the perched water along the cross section.

2.5.1.2 Percolation Fluxes and Fracture-Matrix Partitioning

The percolation flux, or darcy velocity (m/s or mm/yr), of water is defined as the mass flow rate divided by both the cross-sectional area of flow and the density of water. This quantity is important in waste package models for determining the rate of potential radionuclide releases. It also provides a measure of the potential for a region to transmit radionuclides rapidly between the repository and the water table.

For the purposes of TSPA-VA, the repository was divided into six subregions Figure 2-93. These subregions were used to represent different groupings and categories of waste packages in near-field and waste-package models. Thermal hydrology calculations differentiated between these six subregions to produce temperature and relative humidity plots corresponding to each sub-region. The purpose of this section is to describe ambient fracture percolation fluxes (distributions and averages) that correspond to each of the six subregions for the base case.

Histograms of the fracture-percolation flux over each of the six subregions are shown in Figure 2-94 for the base-case simulations with present-day infiltration (mnaqb_p). Results show that regions near the center of the repository (CC, SC, and NW) have the highest percolation fluxes, which reflect the higher infiltration rates at the surface. The average fracture percolation flux is around 11 mm/yr in subregions CC and SC, but only around 4–5 mm/yr towards the eastern part of the repository in NE and SE. Similar trends in the distributions are seen in the other base-case simulations. Table 2-40 shows the mean percolations fluxes for several base-case simulations. It is interesting to note that the mean percolation fluxes in several of the subregions in the highest infiltration scenarios are over 300 mm/yr.

A spatial distribution of percolation flux and the partitioning of flow between fractures and matrix can be observed in Figure 2-95 through Figure 2-99 for the base-case simulation with mean present-day infiltration. Figure 2-95 shows the infiltration along the top surface of the three-dimensional model. This map is consistent with the present-day infiltration map shown in Figure 2-18 and is provided as a reference for the following figures. Figure 2-96 and Figure 2-97 show a plan view of the fracture and matrix percolation fluxes, respectively, at the repository horizon. The flow in the vicinity of the repository is predominantly in the fractures, and very little attenuation (diversion) of the infiltrating mass flow has occurred. It is also interesting to note that a significant amount of flow in the faults (Solitario Canyon, Ghost Dance, and Dune Wash) at the repository horizon is in the matrix. Because the matrix permeability in the faults is very large (see Table 2-24), fast flow can still occur through the matrix in the faults. Figure 2-98 and Figure 2-99 show a plan view of the fracture and matrix percolation fluxes, respectively, at the water table. Note that a significant amount of flow in the fractures in the vicinity of the repository has been attenuated, especially in the northern part of the repository. Figure 2-99 shows that much of the flow that was carried in the fractures at the repository horizon has now transitioned into the matrix. However, the total downward flow (fracture plus matrix) at the water table in the northern part of the repository is still significantly reduced from the total downward flow at the repository horizon. This result is consistent with the presence of perched water below the northern part of the repository, which has the potential to divert downward flow laterally as shown earlier in Figure 2-92.

The partitioning of flow between fractures and matrix can also be quantified in one-dimensional plots of mass flow (normalized to the infiltration rate applied to the column). Figure 2-100 shows the normalized fracture and matrix mass flow rates for simulation mnaqb_p (present-day infiltration, mean fracture alpha) along borehole SD-9. The infiltration is introduced in the fractures at the top of the model domain, but the flow transitions almost entirely to the matrix in the PTn unit. Because the fracture alpha parameter at the top of the TSw unit was reduced to suck water out of the TSw matrix, the flow is once again predominantly in the fractures through the TSw unit. (The use of the downstream weighting, which was used at the interface of vitric/zeolitic interfaces, should also be applied to the interface of the PTn and TSw units in future studies to allow flow to partition back to the fractures without reducing the fracture alpha at the top of the TSw unit. It was not used here because calibrations that used upstream weighting at those interfaces had already been performed.) The flow transitions back to the matrix within the Calico Hills unit, but it should be noted that the total downward flow is significantly reduced (nearly two orders of magnitude) in the lower portions of the model domain. This result is again consistent with the presence of perched water near the top of the

Calico Hills, which apparently diverts flow laterally. Results of other base-case simulations at this location are similar.

Figure 2-101 shows the normalized fracture and matrix mass flow rates for simulation mnaqb_p (present-day infiltration, mean fracture alpha) along borehole SD-12. Because the presence of perched water is reduced in the location of SD-12, the total downward flow is attenuated less toward the bottom of SD-12 relative to SD-9. This further confirms that the presence of perched water in the northern part of the repository diverts a significant amount of flow laterally. Also, note that the downward flow at the bottom of SD-12 has transitioned into the matrix because there is vitric in Calico Hills.

Areal plots of total percolation flux (fracture plus matrix) using the expected base-case with LTA infiltration (mnaqbf1) are shown in Figure 2-102. The total percolation at the repository is nearly the same as the infiltration at the surface, confirming the primarily vertical flow between the surface and the repository as shown in Figure 2-92. However, significantly less percolation reaches the water table in the northern vicinity of the repository, where perched water was shown to divert flow laterally in Figure 2-92. Hence, Figure 2-102 shows large regions of "red" where perched water has diverted percolation. Regions of high percolation ("purple") appear where the diverted water eventually meets the water table, which is about 80 m higher than in the present-day infiltration simulations. Aside from the change in water table elevations, the general flow pattern is similar among the different climate scenarios.

2.5.1.3 Transport from Repository to Water Table

The aqueous travel time between the repository and the water table is also an important facet to performance. The groundwater-travel time can be assessed by tracking tracers from the repository to the water table. Five hundred thousand nonsorbing, nondiffusing particles are released from 360 elements that make up the repository (Figure 2-93) at time zero. Hydrodynamic dispersion was neglected (in the context of not including a physical-dispervisity value in the model). Figure 2-103 and Figure 2-104 show the cumulative breakthrough curves of this unretarded tracer at the water table for the base-case simulations.

Figure 2-103 shows that the infiltration rate, as dictated by the present-day, LTA, and superpluvial-climate conditions, has a significant influence on travel times between the repository and water table. While less than 25% of the particles reached the water table within 1,000 years in the present-day climate, nearly 95% of the particles reached the water table within 1,000 years in the superpluvial climate. The travel time of particles in the LTA climate fell in between those of the present-day and superpluvial climates. The arrival of particles at the water table was bi-modal because the model was of a dual-continuum nature. The earliest arriving particles (as indicated by the "knee" in the curves) were transmitted through the fracture continuum, while the later arriving particles were transmitted in the matrix. Nearly 30% of the tracer particles reached the water table via the fractures in the LTA and superpluvial cases, yielding a rapid travel time of less than 1 year.

Figure 2-104 shows the breakthrough curves for all five base-case simulations using the LTA climate scenario. The infiltration is seen to be the strongest driver for travel time and shape of the breakthrough curves. The variation in fracture alpha does not affect the breakthrough curves significantly for the unretarded tracer used in these analyses. However, sensitivity studies with matrix diffusion ~10^{-11} m^2/s show some sensitivity of the breakthrough curves to the various fracture alphas.

2.5.1.4 Guidance for Sensitivity Studies

Based on the foregoing results, it is evident that infiltration plays a dominant role in the resulting percolation fluxes and travel times beneath the repository. Therefore, additional simulations have been performed that investigate wider ranges of infiltration (times 5 and divided by 5). In addition, based on parameter sensitivity studies performed in Section 2.4.3.2.3, the calibration of additional property sets has been performed and is discussed in Section 2.6.1. Results indicate that increased infiltration directly increases percolation fluxes and decreases travel times beneath the repository. More details are given in Section 2.6.1.1.

2.5.2 Seepage

2.5.2.1 Percolation Values

As described in foregoing sections, the UZ-flow base case for TSPA-VA consists of fifteen site-scale flow fields, as listed in Table 2-37. However, the seepage base case was developed in parallel with development of the UZ-flow base case, and the initial determination of what percolation-flux range to use, etc., was made using an earlier version of the UZ flow, called the "preliminary base case," which is described further in Section 2.6.1.1.1. The preliminary-base-case flow fields are nearly the same as the base-case flow fields, except that a wider range of infiltration uncertainty was assumed—ranging from the base infiltration divided by five up to base infiltration multiplied by five rather than from base divided by three up to base times three. In addition, the preliminary base case did not include systematic variations of fracture alpha, so that there were only nine flow fields (three infiltrations times three climate states).

In order to run the seepage model for the appropriate range of percolation values, we looked at the distribution of percolation rates over the repository area for the nine preliminary-base-case flow fields produced by the site-scale model. Figure 2-105, Figure 2-106, and Figure 2-107 show histograms of the percolation flux at the repository for the three base-infiltration flow fields, which are denoted Qb, Qb_f1, and Qb_f2 (refer to Table 2-57). These figures show that percolation is quite variable over the repository. Summary statistics for the distributions shown, plus those for the other preliminary-base-case flow fields, are shown in Table 2-41 (refer to Table 2-57 for nomenclature). To conservatively capture the behavior at the high end of the flux range, we ran the seepage model for flux values at the 95th percentile level rather than mean values. The percolation values chosen for analysis are 14.6 mm/yr, 73.2 mm/yr, and 213.4 mm/yr. In addition, based on the results of those runs, 500 mm/yr was chosen as a fourth percolation value to analyze.

2.5.2.2 Fracture α and k Values

As already discussed, there are no actual measurements of fracture-hydrologic properties. All values that are used are based on conceptual models or analogs, and it is uncertain how well they represent the actual behavior of the UZ at Yucca Mountain. As discussed in Section 2.4.3.1.2, the conceptual model being used here to derive values for fracture α is based on the capillary-rise equation and measurements of air permeability and fracture density. For the three repository units—tsw34, tsw35, and tsw36 (the Topopah Spring Middle Nonlithophysal, Lower Lithophysal, and Lower Nonlithophysal, respectively)—the range of calculated α values is typically about an order of magnitude or so (see Section 2.4.2.1). Thus, we decided to use a range of one order of magnitude centered on the primary value. Specifically, the seepage model was run for α values of 3.3×10^{-4}, 9.7×10^{-4}, and 3.3×10^{-3} Pa^{-1}. The relative weights of the three values were set to 0.25, 0.5, and 0.25, respectively. This choice is somewhat arbitrary, but reflects a desire to allow significant probabilities for the outlying values, while giving the primary value preference.

The geostatistical heterogeneity model already includes spatial variability of fracture permeability, of course, but there is also a larger-scale component of the heterogeneity. For example, the borehole air-permeability tests typically indicate permeability values about an order of magnitude lower than those indicated by the pneumatic-calibration work (in TSw). One possible explanation for this discrepancy is that the higher pneumatic-calibration values represent the permeability of very large fractures and features that may have average spacing of tens of meters or more. Thus, they are not very representative of typical conditions at the drift scale and one does not want to base the drift-scale model on them. Even aside from the very-large-scale pneumatic-calibration permeabilities, there is significant variability in measured borehole air permeabilities. The standard deviation in log space is typically about 0.5 or so for TSw (see Section 2.4.3.1.2). Based on this, the seepage model is run with a range of two orders of magnitude in the mean fracture permeability, representing two standard deviations on either side of the primary value. The actual values used were 10^{-14}, 10^{-13}, and 10^{-12} m^2. When using the values other than the primary value, the same heterogeneity structure was used (depicted in Figure 2-55), with all permeability values simply scaled up or down by a factor of ten. The relative weights of the three values were set to 0.25, 0.5, and 0.25, respectively, with the same reasoning as above. The values used for the model runs and the relative weights are summarized in Table 2-42 (the sum of each row or column adds up to the weights given above).

It is important to note that we treat these ranges of values as uncertainty, not as spatial variability. Certainly there is both, but our conceptual model is that the combinations in Table 2-42 represent the uncertainty in the values, while spatial variability is represented by the geostatistical variations described in Section 2.4.4.2.1.

2.5.2.3 Model Results

The base-case seepage model (three-dimensional, heterogeneous fracture k, X_{fm}=0, steady state) was run for the matrix of cases shown in Table 2-42, for the four percolation rates listed above in Section 2.5.2.1. Each case was run for three geostatistical realizations (the three "parts" described in Section 2.4.3.2.1) in order to encompass more of the variability of the system. Thus, a total of $9 \times 4 \times 3 = 108$ three-dimensional simulations were run with TOUGH2. The results are tabulated in Table 2-43 through Table 2-53. For each combination of parameters, three seepage rates are given, for three 5-m drift segments, representing three waste-package-sized areas. Thus, the seepage rate represents the amount of water that could contact a waste package if it were placed there.

Some important points about the results are:

1. The numbers given are percentages of the percolation flux flowing in the top boundary over a 15-m-long area the width of the drift. Thus, the actual seep flow rate is given by the percentage listed (divided by 100), times the percolation rate q, times an area of 75 m^2, (15 m × 5 m).

2. The seepage percentages are given two ways: In Table 2-43a, Table 2-44a, etc. are given the seepage into the top half of the drift (from spring line to spring line). In Table 2-43b, Table 2-44b, etc. are given the total seepage into the drift. The difference is the amount that seeped into the bottom half of the drift, which happens sometimes if there is a low-permeability obstruction that channels water toward the lower part of the drift. The total seepages are given for information, but only the seepages into the top half of the drift are used for input to the rest of the TSPA. The reasoning for this is simply that water seeping in the side of he drift would not be able to drip onto a waste package.

3. A waste package is only about 1.5-m wide, but we are counting all seepage from a 5-m-wide area as potentially contacting a waste package. This choice should be conservative. It is intended to cover some effects that have not been explicitly included in our model such as drift collapse and backfill that could spread out an incoming plume.

2.5.2.4 Distributions for f_s and Q_s

From the tables of results in the previous section, project personnel derive appropriate distributions of seepage fraction (fraction of waste packages contacted by seeps, denoted by f_s) and seep flow rate (flow rate of water onto a waste package that is contacted by one or more seeps, denoted by Q_s), for use by the near-field, waste-package, and waste-form components of the TSPA. These distributions, which vary as functions of percolation flux, constitute the base-case abstracted seepage model for TSPA-VA.

To begin, Table 2-55 gives summary statistics for the distributions defined by the seepage rates in Table 2-43a through Table 2-53a combined with the weighting factors in Table 2-42. The distributions from which to sample f_s and Q_s by applying these statistical descriptors to beta probability distributions are defined. A beta distribution is uniquely specified by a minimum, a maximum, a mean, and a standard deviation. For f_s, the minimum and maximum are obviously 0 and 1. For Q_s, the minimum is again 0, but there is no obvious choice for the maximum. However, if the maximum is set to a large value, it will not affect the distribution significantly in the part of the distribution that is actually being sampled. That is, the maximum value will affect the shape of the distribution only far out on the tail, at probability values that are very unlikely to be sampled when 100 or 1,000 samples are drawn. Thus, we set the maximum value of the Q_s distribution to be 10 standard deviations above the mean.

An example of a beta-distribution fit to the calculational results is shown in Figure 2-108, which shows a cumulative distribution function (CDF) defined for f_S at q=73.2 mm/yr along with the beta distribution defined by the mean and standard deviation. Considering that there are only a few data points (one f_S value for each hydrologic-property set in Table 2-42—f_S is just the fraction of the drift segments that have some seepage), the beta distribution fits the CDF reasonably well.

Since we have results for only a few percolation fluxes, we must specify how to extend the distribution definitions to other fluxes. For percolations within the range of the calculational results, the simplest choice is to use linear interpolation between the points. Above the range, we extrapolate linearly. Fortunately, it is only for the superpluvial climate applied to the high-infiltration case (i.e., flow field Qbx5_f2) that percolations ever get that high. Below the calculational range (i.e., below 14.6 mm/yr), if the mean Q_S values are extrapolated linearly they go to zero at 7.2 mm/yr. The standard deviation of Q_S extrapolates to zero at 7.9 mm/yr. Thus, for the calculational model of seepage being used, and with the parameter values and weightings being used, there is a threshold for seepage into drifts at about 7 mm/yr. Since it does not make much difference, we opted to take the lower of the two numbers, 7.2 mm/yr, as the threshold for the initial abstracted model. Note that if the mean goes to zero the standard deviation must as well, because any Q_S values greater than zero would imply a mean greater than zero. Note also that if Q_S goes to zero, implying no flow into drifts, then f_S must go to zero as well.

It is important to consider, however, how the abstracted seepage model is used. For the engineered-barrier-system calculations, the repository is divided into six regions (see Figure 2-93). In each region, the average fracture flux at the repository is calculated and used in the abstracted seepage model to determine the fraction of waste packages affected in that region and the water-flow rates onto those waste packages. (Only the fracture flux is used because matrix flow is not expected to seep into drifts and because the process-based seepage calculations were made with a fracture-only model.) The seepage threshold mentioned above is problematic within this method, because even though the average flux in a region is lower than the threshold there may be locations within the region that have flux above the threshold (see Figure 2-105, for example, which has a mean percolation very near the threshold but which shows that some locations have fluxes much higher than the threshold and others are below the threshold).

To address this problem, we took histograms of fracture flux at the repository horizon for each of the six repository regions, for the three lowest-infiltration cases (Qbd5, Qbd5_f1, and Qb). The initial abstracted seepage model described above (mean and standard deviation taken from Table 2-55, with both going to zero at 7.2 mm/yr and linear interpolation between values) was applied to each percolation in the histogram and the resulting average and standard deviation of f_S and Q_S were calculated, along with the average q. The results are shown in Figure 2-109 and Figure 2-110. The figures show lines for the initial abstracted seepage-model quantities, which go to zero at 7.2 mm/yr. The values calculated from the percolation histograms are also shown, and it can be seen that they are close to the initial lines for fluxes above about 9 mm/yr, but deviate significantly at lower fluxes. We conclude from this that the model does not require a correction for the spatial variability of percolation flux except at the low end. To make this correction, we add three of the new points, which envelop the other points, to the abstracted model, including an adjusted threshold value of 2.2 mm/yr.

The points added to the initial model, both for low percolations and high percolations, are shown in Table 2-56 (note that when the mean f_s goes to one, its standard deviation must go to zero because any f_s values less than one would imply a mean of less than one). The means and standard deviations for the base-case abstracted seepage model are plotted in Figure 2-111 and Figure 2-112. Figure 2-113 and Figure 2-114 illustrate the ranges of the distributions as they vary with percolation flux. Of particular note is that the seepage-fraction distribution is very wide over much of the percolation range, reflecting the great variability of the seepage process.

2.5.2.5 Thermal Perturbations

Repository heating will have a significant effect on seepage, at least for a period of time. During the boiling period there will be little or no seepage into the emplacement drifts, and before and after the boiling period seepage may be enhanced because of condensate drainage (Nitao 1997a, pp. 1-8). In addition, there could be permanent changes to seepage because of accumulation of mineral precipitates above the drifts or because of collapse of the drifts.

The only one of these effects that is included in the TSPA-VA base case is the reduction of seepage during the boiling period (based on the results of Nitao 1997a, pp. 1-8), and it is included by reducing seepage to zero when the drift-wall temperature above a waste package is above the boiling temperature. The other effects are more difficult to model, but consideration of them is recommended to obtain a more defensible model. A possible abstraction for thermal-hydrologic effects of seepage is discussed in Chapter 3 (Section 3.6.5) of the Technical Basis Documents.

2.6 SENSITIVITY STUDIES

2.6.1 UZ Flow

Sensitivity analyses have been performed to complement the base-case model presented in Section 2.5.1. The bases for these alternative models have been discussed in Section 2.4.3.2 and are summarized here. From parameter-sensitivity results reported by Bodvarsson et al. (1997, Chapter 7) and from additional sensitivity studies presented in Section 2.4.3.2, the key UZ-flow parameters are the infiltration, the fracture-matrix connection-area reduction factor, and the fracture van Genuchten alpha parameter. Also potentially important are matrix and fracture permeabilities, and the fracture van Genuchten *m* parameter (plus, for transport and possibly for TH, the fracture porosity), but these parameters appear to be less important than the first three above. As a result, additional sensitivity studies have employed the following:

- A wider range of infiltration rates (times 5 and divided by 5) was examined using the LBNL site-scale UZ-flow model. Parameter sets were calibrated to these different infiltration rates, and the percolation rates and travel times were compared to the base case.

- A second alternative UZ-flow model, the DKM/Weeps model, was defined that is similar in behavior to the Weeps model, which was used in TSPA-1991 (Barnard et al. 1992, 4.31 through 4.53) and TSPA-1993 (Wilson et al. 1994, Chapter 15, pp. 1-70). Measured and inferred values for all matrix and fracture hydraulic properties were used, and the fracture/matrix reduction factor was set equal to upstream relative permeability (Ho 1997, pp. 401-410; Bodvarsson et al. 1997, Chapter 7). If the fit to matrix-saturation data was not sufficiently good with this simple choice, the X_{fm} value was scaled up or down globally to get a reasonable fit to the data. There are two aspects of the DKM/Weeps alternative model that provide useful insights into repository performance. First, the DKM/Weeps model has more fracture-dominated flow than the base case, including the nonwelded layers, so it shows whether repository performance is adversely affected by a much greater fast-flow component than exists in the base-case model. Second, having X_{fm} as a dynamical variable that depends on the flow, rather than as a fixed factor, could lead to differences in behavior when climate changes (and during the thermal period in thermohydrological models).

- The matrix permeabilities in the Calico Hills zeolitic units have been varied from the statistical mean. This parameter was thought to have a significant influence on travel times from the repository to the water table, so their values were increased and decreased by one standard deviation to determine the potential effects on UZ transport.

The following sections present more details on the development and results of the above sensitivity analyses.

2.6.1.1 Infiltration Sensitivity Study

In this section, a set of simulations using a wider range of infiltration rates than those used in the base case is presented. A description of the parameter calibration for these simulations is provided, and the results are compared to the base case.

2.6.1.1.1 Property sets for infiltration sensitivity study

The property sets that were calibrated for the current sensitivity study were actually created before the development of the base case described in Section 2.4.3.1.4 above and were intended for use in TSPA-VA calculations. As a result, they were deemed the "preliminary base case." The primary difference between the preliminary base case and the base-case property sets (Table 2-19 through Table 2-23) is in the treatment of the van Genuchten fracture alpha (air-entry) parameter. In the preliminary base case, these parameters were estimated using calibration, but in the base-case property set, these values were prescribed as described in Section 2.4.3.2.2 to limit the degrees of freedom during calibration. Because the values of fracture van Genuchten parameters prescribed in the base case were more realistic than the calibrated values of the preliminary base case (Section 2.4.3.2.2), the preliminary base case was used only as a sensitivity analysis. The development of all other parameters aside from the fracture van Genuchten alpha parameter is identical to the process described in Section 2.4.3.1.4 above for the base case.

Three property sets were calibrated using the present-day infiltration, the present-day infiltration divided by five, and the present-day infiltration multiplied by five. Together with the LTA and superpluvial climate scenarios for each present-day scenario, a total of nine simulations were run as shown in Table 2-57 and Figure 2-115. The preliminary base-case parameter sets used in this infiltration sensitivity study are shown in Table 2-58 through Table 2-60.

2.6.1.1.2 Results of Infiltration Sensitivity Study

The hydrologic behavior resulting from the parameter sets used in this sensitivity study are nearly identical to the base-case simulations for the same infiltration rates. The predicted ambient saturations generally match well with observed borehole saturations, and flow patterns are the same as those shown for the base case in Figure 2-102. The partitioning of flow also behaves similarly to the base case; nearly all of the water is carried in the fractures of welded units and in the matrix of the nonwelded units as indicated in Figure 2-100 and Figure 2-101.

Table 2-61 shows the average fracture-percolation fluxes over the six repository subregions for each of the nine sensitivity runs shown in Table 2-57. The percolation values for the present-day infiltration cases are identical between the base case and the sensitivity run. However, as expected, the percolation values for the high and low bounds of the infiltration sensitivity runs are greater and lower, respectively, than the bounds of the base case. The nearly vertical flow above the repository results in a nearly direct mapping of the surface infiltration to the percolation flux at the repository. As a result, the case with superpluvial infiltration rates times five has approximately five times greater percolation values than the base-case superpluvial values. The influence of these extreme percolation values on travel times between the repository and the water table is presented in Figure 2-116. A total of 500,000 unretarded particles (no matrix diffusion, no dispersion) were released as a pulse uniformly over each node within the six repository subregions shown in Figure 2-93. The median breakthrough time for the superpluvial-times-five case is approximately 20 years, whereas the median breakthrough time for the present-day-divided-by-five case is over 10,000 years. This range of travel times is similarly captured by the base-case simulations presented in Section 2.5.1.3, although to a slightly lesser extent. Therefore, because current studies of infiltration indicate that the maximum present-day infiltration should not exceed a factor of three times the current present-day infiltration values (Section 2.4.2.9), the times-five and divided-by-five cases examined in this sensitivity analysis were not used in TSPA-VA.

2.6.1.2 DKM/Weeps Alternative Model

As introduced earlier, the DKM/Weeps model yields more flow through fractures throughout the entire unsaturated system, most notably in the nonwelded units. A significant reduction in the fracture/matrix conductance allows more water to stay in the fractures without being imbibed into the matrix. The reduction factor, as described in Ho (1997, pp. 401-412), consists of the upstream relative permeability for liquid flow. To aid in the calibration of the model to matrix saturations, a global X_{fm} is also used as an additional fitting parameter.

Sensitivity analyses described in Section 2.4.3.2.3 provided sensible ranges for the most sensitive parameter (fracture permeability) in the DKM/Weeps model. All other hydrologic properties in the DKM/Weeps model are based on direct property measurements (e.g., saturated matrix permeability) or on parameters inferred from direct measurements (e.g., van Genuchten's alpha parameters for fractures calculated from fracture permeability and frequency data through the cubic law (Domenico and Schwartz 1990, pp. 86-87) and capillary theory) (Wu et al. 1998, pp. 32-33 and 43). A matrix of five runs that included uncertainty in present-day infiltration and fracture permeability was developed and is shown pictorially in Figure 2-117. Together with the LTA and superpluvial-climate scenarios for each present-day scenario, 15 runs were performed. Table 2-62 summarizes the runs and the nomenclature associated with each of the runs. The five parameter sets calibrated to the present-day infiltration scenarios using the DKM/Weeps model are shown in Table 2-63 through Table 2-67.

2.6.1.2.1 DKM/Weeps Results

The predicted liquid saturations at SD-9 and SD-12 are shown in Figure 2-118 and Figure 2-119, respectively. Because the DKM/Weeps matrix permeabilities were not calibrated, the slightly lower values that were measured cause the matrix liquid saturations to be higher than in the base case. The predicted saturations for the other DKM/Weeps simulations are similar. Nevertheless, the general match between the predicted matrix saturations and the observed borehole saturations is comparable.

Table 2-68 gives the mean fracture-percolation flux over each of the six repository subregions for nine representative cases of the DKM/Weeps runs (see Table 2-62 for nomenclature). Similar to the base case, the infiltration was found to be the most sensitive parameter in changing the magnitude of percolation over each of the repository subregions. The variation of the fracture permeability did not have a significant effect on the percolation values at the repository because, in both cases, the flow in the vicinity of the repository was predominantly in the fractures. As shown in Table 2- 68, the values of the percolations fluxes are quite similar to those of the base case.

The primary difference between these two models is in the partitioning of flow between fractures and matrix in the nonwelded units. Figure 2-120 through Figure 2-123 show the fracture- and matrix-percolation flux at the repository and at the water table for the DKM/Weeps run with mean present-day infiltration (kmnqb_p). The fracture- and matrix-percolation flux at the repository is nearly identical to that of the base case. However, there is an increased amount of flow in the fractures at the water table in the DKM/Weeps simulation as compared to the base case in particular regions (Figure 2-98 and Figure 2-122). The increased partitioning of flow in the fractures can be quantified in one-dimensional plots of fracture and matrix flow as a function of elevation along SD-9 and SD-12 (Figure 2-124 and Figure 2-125, respectively). The flow through the nonwelded PTn unit at SD-9 is almost entirely in the fractures using DKM/Weeps; in the base case, the flow is almost entirely in the matrix. Below the repository at SD-9, the total flow is greatly attenuated because of the presence of perched water. At SD-12, the flow through the nonwelded PTn unit is predominantly in the fractures using DKM/Weeps. This contrasts the predominantly matrix flow in the PTn unit at SD-12 for the base case. Below the repository at SD-12, the DKM/Weeps model yields a nearly equal partitioning of flow between the fractures and matrix in the Calico Hills unit. The base case resulted in predominantly matrix flow in the Calico Hills unit below the repository at SD-12. In some locations toward the center of the repository, the DKM/Weeps model yields predominantly fracture flow throughout the entire UZ.

Figure 2-126 shows tracers that were released as a pulse at two surface locations (10 particles at each location) above the left and right ends of the repository along two east-west vertical cross-sections (N235,000 and N233,400). The LTA infiltration scenario was used with the mean fracture permeability (kmnqbf1). The open symbols denote a higher concentration of the tracer in the fracture, while the solid symbols denote a higher concentration in the matrix. The movement of the unretarded tracers for the DKM/Weeps simulation is similar to that of the base case shown in Figure 2-92, but the partitioning of flow between fractures and matrix is different. In the PTn, the tracers are partitioned more in the fractures in both cross-sections than in the base-case simulations. Also, flow beneath the repository in the DKM/Weeps simulations shows more fracture flow, although the partitioning is not as pronounced as in the PTn unit. Lateral diversion caused by perched water still exists in the north cross-section, and flow patterns are very similar between the DKM/Weeps and base-case simulations.

The consequence of the increased fracture flow can be seen in Figure 2-127, where the breakthrough curves of a pulse of unretarded tracer released at the repository using the DKM/Weeps simulation (kmnqb) are presented. Compared to the results of the base case, the travel times are much shorter as a result of increased transport through fractures in the DKM/Weeps simulation. Nearly 50% of the tracer exhibits an early arrival (less than 1 year) via fractures during the superpluvial and LTA climates, and approximately 40% of the tracer experiences early arrival during the present-day climate. This has important consequences for repository performance during times less than 10,000 years. The fast transport of radionuclides through fractures using the DKM/Weeps model increases the dose rates at times less than 10,000 years when compared to the base case; however, for longer times (~100,000 years), the effect of rapid transport through fractures does not significantly impact the long-term dose.

The effects of varying fracture permeability on the DKM/Weeps model is shown in Figure 2-128. The breakthrough curves for all long-term-climate scenarios using the DKM/Weeps model are presented. Unlike the base case, the parameter variation has a significant effect on the travel time in addition to the infiltration variation. Runs with the maximum permeability (see Table 2-35 for range of fracture permeabilities used in DKM/Weeps simulations) show a significant amount of transport through the fractures. For the case using LTA infiltration multiplied by three (I*3) and a maximum fracture permeability, over 90% of the tracer arrives at the water table within 1 year. The same infiltration combined with a minimum fracture permeability results in 60% of the tracer arriving at the water table within 1 year. A similar disparity is observed in Figure 2-128 when the long-term-average infiltration is divided by a factor of three (I/3) and a range of fracture permeabilities is used.

The increased flow through the fractures also allows a fast component of flow between the surface and repository. As emphasized by the Performance Assessment Peer Review (PAPR) Panel, isotopic evidence (bomb pulse) indicates that travel times between the surface and some portions of the ESF can be less than 50 years (Fabryka-Martin et al. 1998, pp. 93-96). The exact disposition of these fast flow paths is unclear, but the existence of bomb pulse at the repository horizon appears to be more concentrated near faults. Figure 2-129 shows the paths of unretarded tracer released from the surface along a vertical east-west cross-section through the center of the repository (N233,400 m). The tracer was released as a pulse (100 particles at 5 surface locations), and the paths of the tracer during a 50-year period were recorded as indicated by the locations of the symbols in the plots. In the DKM/Weeps simulation, the tracer has reached the repository (shown as a solid line) at all locations. In the base-case simulation, the tracer only reaches the PTn unit in 50 years over most of the repository. Near the Solitario Canyon fault, which borders the west end of the repository, the tracer has propagated past the repository horizon in the base-case simulation. The observation of increased bomb pulse near faults is consistent with the predicted behavior of the base-case model, but the existence of bomb pulse in regions away from faults is not predicted by the base-case model. In contrast, the DKM/Weeps model predicts that fast paths can occur at all locations. It is important to note that Figure 2-129 does not indicate that all of the particles in the DKM/Weeps model have propagated past the repository horizon during the 50-year period. The figure just shows all locations where a particle has resided at any point in time.

2.6.1.3 Zeolitic Matrix Permeability

Additional flow fields were generated using the three-dimensional UZ site-scale model to evaluate the sensitivity of the model to the matrix permeabilities used for the zeolitic layers. The base-case simulation using LTA infiltration (mnaqbf1) was used as the reference case. Each model layer, including layers ch1zc, ch2zc, ch3zc, ch4zc, pp2zp and bf2zp, was altered by increasing and decreasing the existing matrix permeability of each layer by one standard deviation. Other rock properties were not re-calibrated with the modification of the zeolitic matrix permeabilities. The standard deviations used are the ones listed in Table 5.2.2 of Wu et al. 1998, pp. 24-26) and are also listed in Table 2-69 of this document. Steady-state hydrologic conditions were obtained using the EOS9 module of TOUGH2 as described in Section 2.4.3.9 for cases in which the zeolitic matrix permeability was increased and decreased by a standard deviation.

Figure 2-130 shows the breakthrough of a tracer at the water table released as a pulse (500,000 particles) uniformly over the repository for the base-case LTA simulation. Figure 2-130(a) shows the results for an unretarded tracer (no matrix diffusion, no sorption), while Figure 2-130(b) shows the results for a tracer with a sorption coefficient (Kd) of 2.5 cc/g in the zeolitic-matrix units. For the simulations with an increased zeolitic-matrix permeability, the breakthrough curve exhibits longer travel times. The increased zeolitic-matrix permeability allowed more flow to occur through the matrix (note the slightly lower fraction of particles that arrive at early times through fractures); thus, more particles were transported (at slower rates) through the matrix. The delay associated with increased zeolitic-matrix permeabilities is most notable when sorption occurs in the zeolitic-matrix as shown in Figure 2-130(b). Decreasing the zeolitic matrix permeability did not change the breakthrough curves significantly. A decrease in the zeolitic matrix permeability causes more flow to be diverted in the zeolitic fractures (yielding shorter travel times), but because the partitioning of flow was already predominantly in the fractures, the impact of decreasing the zeolitic-matrix permeabilities was small.

2.6.2 Seepage

Three sensitivity analyses were conducted in which the weightings in Table 2-42 were modified. Two kinds of modifications to the seepage-model inputs are made. One is to narrow the fracture-property distributions (i.e., assume that the fracture properties have less uncertainty than in the base case) and the other is to skew the distributions toward higher or lower fracture apertures.

As discussed previously, three values of fracture permeability (k_f) and three values of fracture alpha (α_f) were used in the drift-scale flow simulations that were performed to calculate the amount of seepage into emplacement drifts. The base-case weights for both parameters were assigned as (0.25, 0.5, 0.25); that is, the lowest value was weighted 25%, the middle value 50%, and the highest value 25%. The middle value is the preferred value, based on the available data, and the low and high values were chosen to span a reasonable range based on the variability in the data. For the first sensitivity analysis, the weights of the outlying values were cut in half, giving weights of (0.125, 0.75, 0.125). These weights emphasize the best-estimate parameter values considerably more. They are also reasonable, given what is known about fracture properties. Taking fracture permeability as an example, the base-case weights imply a log standard deviation (i.e., the standard deviation of the logarithm of permeability) of 0.7, while the narrower distribution implies a log standard deviation of 0.5. These standard deviations are near the low and high ends of the observed range for air-permeability measurements in the repository host rock (see Table 7.11 of Bodvarsson et al. 1997).

This modified set of weights was applied to the process-model results to generate new seepage distributions, and then TSPA calculations were run with the modified seepage distributions. The modified statistics for f_s and Q_s are shown in Figure 2-131 and Figure 2-132.

The other two sensitivity analyses have modified weights that represent systematically smaller or larger fractures. These cases could approximate the possibility of smaller or larger fracture apertures caused by thermal-hydrologic-chemical or thermal-hydrologic-mechanical processes. Smaller fracture apertures imply both lower k_f and lower α_f, because α_f is proportional to the effective fracture aperture and k_f is proportional to the cube of fracture aperture. Therefore, to simulate smaller fracture apertures, the weights for the parameter values were shifted to smaller values, giving (0.67, 0.33, 0) as the low, middle, and high parameter values. Similarly, to simulate larger fracture apertures the weights were changed to (0, 0.33, and 0.67). The resulting seepage parameters are plotted in Figure 2-133 through Figure 2-136.

2.7 SUMMARY AND RECOMMENDATIONS

This chapter has detailed the development of four major components of UZ flow: (1) climate, (2) infiltration, (3) mountain-scale UZ flow, and (4) drift-scale seepage. Issues associated with each component have been presented, along with abstraction/testing plans that addressed these issues. The bases for the development of climate and infiltration models, UZ flow models, and seepage models were discussed, along with a number of sensitivity analyses to investigate relevant processes and parameters. Results for the base-case UZ flow and seepage simulations were then presented, and a series of sensitivity analyses were also discussed. The following sections summarize each of the four major UZ-flow components. The impact of each component on performance, along with guidance and recommendations for license application, are also provided.

2.7.1 Climate

The primary purpose of climate modeling was to provide precipitation rates and water table elevations that varied as a function of future climates. Future climate was modeled in TSPA-VA as a sequence of discrete steady states. Only three discrete climate states were considered for

TSPA-VA: present-day, LTA, and superpluvial. Present climate represented relatively dry, interglacial conditions, while the LTA represented an average pluvial period at Yucca Mountain. The superpluvial represented periods of extreme wetness. The MAP for the present, LTA, and superpluvial climates were estimated to be 150, 300, and 450 mm/yr, respectively, as shown in Table 2-5. These values were used by infiltration modelers to determine appropriate analog sites that had average precipitation rates that were commensurate with the predicted future climate values. The water-table rise from the present-day level (~730 m) was estimated to be 80 m and 120 m for the LTA and superpluvial climates, respectively. The duration of each cycle is tabulated in Table 2-7, but sensitivity analyses have shown that the overall performance is not sensitive to the duration of the climate cycles. The most significant impact was found to be the abrupt changes in water-table elevation and groundwater flow rate that occurred at the transition between climates. Section 2.4.1 provides more details of the climate modeling, and additional information on the development of the climate models can be found in CRWMS M&O (1998, Section 4).

2.7.1.1 Implications for Performance

Climate models strongly impact performance through their influence on precipitation and evapotranspiration. These factors, in turn, influence the predicted infiltration in the UZ-flow model. Therefore, the magnitude and timing of the prescribed climate states is important to performance.

2.7.1.2 Guidance for License Application

Additional work is needed to understand the natural variability of current and future climates for Yucca Mountain. In particular, the adequacy of three distinct climate states needs to be addressed further. If distinct climate states are used in future analyses, their number, timing, duration, and the abruptness of the transition between them need better support. Additional modeling is needed to determine how the dose-rate pulses depend on the time of transition between climates, and whether noninstantaneous transitions would lead to lower peak doses. Appropriate climate analogs need to be defined, based on temperature and other factors in addition to precipitation. The superpluvial climate, especially, needs better definition.

2.7.2 Infiltration

Infiltration modeling provides the spatial and temporal distribution of net infiltration as an upper boundary for site-scale UZ-flow models in TSPA-VA. Distributed net infiltration rates were determined for each of the three climate states using the YMP infiltration model described in Section 2.4.2 (also presented in CRWMS M&O 1998, Section 5.3.4.1). The infiltration model simulated water movement at the ground surface by solving water mass balances using precipitation, a model for evapotranspiration, and available water in the soil profile. Also considered in the model were ground surface elevation, slope, bedrock geology, soil type, soil depth, and geomorphology. The primary driver for the infiltration model was precipitation, which was input using available records or, in some cases, a stochastic model. Daily precipitation records from different locations were used to define the present-day, LTA, and superpluvial climates in the infiltration model. The sites were chosen based on how well their MAP values matched the estimated values associated with each climate. Table 2-10 summarizes the location of the analog sites and the measured and predicted values of precipitation. General results of the infiltration model are as follows:

- The modeled infiltration is highly heterogeneous and clearly correlated with topographic features
- The highest net infiltration occurs along Yucca Crest
- Net infiltration is lower in washes.

The spatially distributed infiltration maps were then upscaled to the site-scale UZ-flow model by averaging the simulated infiltration values over each surface element in the UZ-flow model. Figure 2-18, Figure 2-19, and Figure 2-20 show the infiltration maps for the present-day, LTA, and superpluvial climate scenarios. The average infiltration for each climate over the UZ-flow model domain are 4.9, 32.5, and 118 mm/yr, respectively.

Sensitivity analyses were also conducted to determine the effects of episodic infiltration on the percolation at the repository horizon (Section 2.4.2.8). Results showed that the PTn unit effectively damped episodic pulses that were simulated on a yearly cycle, preventing the transient pulses from significantly impacting the percolation at the repository horizon.

Additional sensitivities that used infiltration to estimate the temperature profile in a borehole indicated that infiltration rates that were greater than three times the average present-day infiltration rate did not allow good matches with observed borehole temperatures because of increased advective heat transfer. Therefore, a factor of three was used as the upper and lower bounds for the range of infiltrations considered in each climate scenario (see Figure 2-52).

2.7.2.1 Implications for Performance

Infiltration strongly influences repository performance because of its influence on mountain-scale unsaturated-zone flow and seepage into drifts (which subsequently affects waste-package-degradation models). The infiltration rates used in TSPA-VA are significantly higher than in past TSPAs. Higher infiltration rates, in general, tend to adversely impact total performance. However, the increased infiltration must be considered in conjunction with other TSPA components such as seepage to understand the overall impact on performance.

2.7.2.2 Guidance for License Application

The greatest need for improvement is explicit inclusion of processes that should be different for future climates, including effects of temperature, cloudiness, vegetation type, surface water runoff/run-on, and snow cover. Even for current conditions, some experts in the UZFEE (CRWMS M&O 1997) suggested that runoff and run-on might be more important than is assumed in the infiltration model.

To provide a more quantitative basis for the uncertainty distribution for infiltration, the infiltration model should be run in a stochastic mode (e.g., Monte Carlo simulation) to derive the infiltration uncertainty from the uncertainties in the input parameters of the model.

Finally, analogues with known infiltration, such as Rainier Mesa and Apache Leap, should be used to test and improve the infiltration models and methods.

2.7.3 Unsaturated Zone Flow

The three-dimensional LBNL UZ-flow model has been used to calculate unsaturated-groundwater flow at Yucca Mountain for TSPA-VA. The model implements the dual-permeability formulation for fracture-matrix interactions and consists of nearly 80,000 elements. Hydrologic properties were determined using both direct measurements and calibration with field data (Section 2.4.3.1), which included core samples, borehole log data, in situ water potential and temperature measurements, fracture measurements from the ESF, in situ pneumatic data, air permeability tests, and geochemistry data. A great deal of information on the calibration and details of the LBNL UZ-flow model development was taken from Bodvarsson et al. (1997, Chapters 1-4, 6-8, 10-11, 13, 15, 17-19). In the calibration approach, a number of vertical one dimensional submodels that corresponded to borehole locations were extracted from the three-dimensional model. The code ITOUGH2 was used to perform simultaneous inverse simulations with these one-dimensional models to optimize hydrologic parameters by matching predicted and observed matrix saturations and moisture potentials. The selection of hydrologic parameters that were estimated by inverse modeling were influenced by sensitivity studies (Section 2.4.3.2) that determined important parameters to UZ flow, which included the fracture air-entry parameter, α_f, and the fracture-matrix interaction parameter, X_{fm}. The properties that were calibrated in one dimension were then used in the three-dimensional site-scale model, which included calibrations to perched water. Figure 2-52 shows a tree-diagram of the resulting parameter sets that were used for the base case in TSPA-VA, and Table 2-19 through Table 2-24 show the resulting property values for all materials. Additional tests using geochemical data, infiltration data, and alternative weighting schemes were also performed to improve the three-dimensional model and increase confidence in the methods being used (Section 2.4.3.5 and Section 2.4.3.6).

Results presented in Section 2.5.1 show that the flow through the UZ is predominantly in the fractures for the welded units and predominantly in the matrix for the nonwelded units. High infiltrations resulting from climate changes significantly increased the percolation flux in the vicinity of the repository and decreased the travel time between the repository and the water table. Travel times between the repository and the water table ranged from several days to hundreds of thousands of years (Figure 2-103). The fastest transit times resulted from flow through fractures, whereas the matrix contributed to particle breakthrough at the water table at significantly longer times. Perched water, which has been calibrated in the three-dimensional flow model, diverted vertical flow laterally in the three-dimensional model, especially in the northern part of the repository (Figure 2-92). However, the total travel time of the diverted water was not significantly altered due to the fast flow path through the fractures. Sensitivity results using increased infiltration confirmed the importance of infiltration rates in determining travel times between the repository and the water table. In addition, sensitivity results using the DKM/Weeps alternative model showed that there was more significant fracture flow than in the base case, contributing to faster travel times. Finally, sensitivity studies of the zeolitic matrix permeability showed that increased matrix permeability can result in slower travel times due to increased flow through the matrix. However, decreased matrix permeabilities did not result in significant changes from the base case.

2.7.3.1 Implications for Performance

A significant result of the current TSPA-VA UZ flow calculations relative to earlier TSPAs is that the higher estimates of current and future infiltrations can cause percolation fluxes to be significantly greater and travel times to be significantly shorter. While these effects have a negative impact on performance, the impact of UZ flow in general on the total-systems performance calculations must be determined collectively with other system components. For example, high infiltrations are thought to be adverse to performance, but performance calculations have shown that for a period of time, the high infiltration scenarios show a decrease in dose for a period of time. This counter-intuitive result occurs because the temperatures around the waste package are reduced by the increased infiltration, and the corrosion of the waste packages is reduced.

The use of the DKM/Weeps model produced significantly shorter travel times between the repository and water table because of increased partioning of flow through fractures. As demonstrated in total-systems PA calculations, the decreased travel times increase dose rates for periods less than 10,000 years, but for longer times (100,000 and 1,000,000 years), the rapid transport does not significantly impact performance. At these later times, the travel time becomes small relative to the total simulation time, and the decreased travel time in the DKM/Weeps model is less important. However, colloid-facilitated transport can be enhanced by increased flow and partitioning in fractures.

The uncertainty in matrix permeability in the zeolitic units resulted in travel times that could differ by several thousand years. Sorbing tracers traveling through the zeolitic matrix were retarded more if the permeability was increased, but little difference was observed if the permeability was decreased. Because the matrix permeabilities in low-permeability units is likely to be less than the reported values because of excluded "nondetect" values, the uncertainty associated with matrix permeabilities may not significantly impact overall performance.

2.7.3.2 Guidance for License Application

The most important need in the mountain-scale, UZ flow modeling is a better representation of localized channeling of flow, and in particular, the effects of flow in discrete fractures. Current modeling uses continuum models with very coarse spatial discretization, and the adequacy of this approach is not fully established. There are indications from geochemical and isotopic tracers (chloride concentration, ^{36}Cl-to-chlorine ratio and ^{14}C-to-carbon ratio) that channeling of flow might be important. In addition, geochemical, isotopic, and temperature data should be integrated into the calibration procedure because they provide important information about flow through fractures.

More information is needed about the role of perched water in UZ flow. The current model assumes that the water is perched on a very-low-permeability underlying layer and flow is forced to go around it. Other interpretations are possible, such as mixing within the perched water and matrix flow out the bottom.

Thermal alterations of flow and TH-chemical or TH-mechanical alterations of hydrologic properties are potentially important. In the current TSPA structure, these effects fall under the

TH component, but it is necessary to determine whether there should be a coupling of TH effects on mountain-scale, UZ flow and transport.

Technical recommendations for improvement of the current mountain-scale, UZ-flow model include the following:

- Incorporation of the most recent version of the integrated site model (site geologic framework model)
- More refined numerical grid
- Additional data to gain better estimates of fracture-hydrologic parameters
- Additional imbibition tests of hydrologic properties of the matrix
- Additional measurements of permeability of the zeolitic hydrogeologic units and properties of faults
- Additional studies to better characterize and understand the effects of perched-water bodies
- Creation of heterogeneous property sets that take advantage of the heterogeneous distributions provided by Rautman and McKenna (1997, pp. 1-322) and a stochastic representation of the parameter fields in the site-scale UZ model.

Fracture-flow processes should be further investigated with alternative conceptual models and additional field studies, such as niche and alcove studies, the planned east-west cross drift, and the Busted Butte transport study. Other flow processes that need to be further characterized include flow through faults, flow between disparate units (such as at the Paintbrush nonwelded–Topopah Spring welded and Calico Hills vitric–Calico Hills zeolitic interfaces), and fracture/ matrix interactions. Finally, the process of model calibration can be further improved by developing two-dimensional and three-dimensional calibrations against field data, which may require using parallel computing techniques.

2.7.4 Seepage

The abstracted base-case seepage model was based on a large number of three-dimensional process-model calculations. The process model consisted of a three-dimensional heterogeneous fracture-continuum field presented in Figure 2-55. Three blocks of dimensions 20-m high, 15-m wide and 16.5-m long were evaluated independently within this continuum. The drift was represented by a horizontal open cylinder of diameter 5 m at the center of the lower part of the block (Figure 2-56). Simulation grid cells were defined to be 0.5 × 0.5 × 0.5 m. Fracture properties were obtained from air-permeability tests of the DST in the ESF Thermal Test Alcove 5 and from evaluation of fracture surveys in the ESF. As a conservative estimate, matrix flow was neglected in seepage simulations used for TSPA-VA, and sensitivity studies were performed to evaluate the effects of fracture-matrix interactions. Sensitivity studies were also performed to determine the effects of episodic pulses, variations to hydrologic properties, and grid refinement (Sections 2.4.4.5 through 2.4.4.8).

The process-model results were abstracted by fitting the calculated seepage-fraction (f_s) and seep-flow-rate (Q_s) distributions with beta probability distributions for which the mean and standard deviation are functions of percolation flux in the fractures (also, the maximum in the case of Q_s). The final abstracted models are illustrated in Figures 2-111 through 2-114. The seepage process model has been tested against recent preliminary data from the ESF niche liquid-release tests, and appears to fit them reasonably well. Finally, seepage sensitivity studies were performed to investigate reduced variance of fracture properties and variations to the fracture aperture. Results of the sensitivity are shown in Figure 2-131 through Figure 2-136.

2.7.4.1 Implications for Performance

Seepage into the drifts has a significant impact on performance for several reasons. Seepage controls waste-package degradation because the waste-package material (C-22) corrodes only in the presence of liquid water. Following the creation of openings through the C-22, the seepage volume controls the amount of water that can enter the waste package and dissolve the waste form. The flux of water into and through the waste package in turn controls the release rate of the solubility-limited radionuclides from the waste package. The impact of seepage on overall performance has been found to be important for periods ranging from 10,000 years to 1 million years.

2.7.4.2 Guidance for License Application

A number of additional studies have been identified that can be addressed in the near future (or are already underway) that will produce realistic and useful results for TSPA. They are listed below:

- One of the key factors that control the spacing between drip seepage locations is the correlation lengths of spatial heterogeneity of the rock unit. A further careful study of the fracture distribution along the ESF (Bodvarsson et al. 1997, Chapter 7) should be made to provide estimates of these parameters. Field data from the ESF niche study can also yield important information related to this factor.

- A more comprehensive parameter-sensitivity study should be made, including sensitivity of drift seepage to the width of the permeability probability distribution function and the spatial correlation lengths of the heterogeneous fields. The occurrence of special features, such as long fractures intercepting the drift, should also be studied. The range of situations and property values used should be representative of the three stratigraphic units in which the potential repository will reside.

- For reliable results, the study needs to be performed with more realizations in the sense of a stochastic analysis and with potentially finer grids. Previous sensitivity studies have indicated that seepage may increase with finer grids.

- Gravity-driven flux in near-field discrete fractures close to the drift wall may increase the probability of drift seepage. Additional study of this possibility is needed.

- Further study on successive percolation pulses should be carried out, especially since the current calculations seem to indicate that the time frame for the system to recover to its original initial state after the first pulse is very long, perhaps as long as hundreds of years.

The ESF niche test is an important first step in verifying seepage models, but it is primarily a test of the overall conceptual model of the drift opening acting as a capillary barrier. The test offers little validation of the calculated values of seepage fraction, which the TSPA results show to be the most important aspect of seepage—indeed, the most important aspect of repository performance. Seepage fraction, or the fraction of waste packages contacted by seepage water, is related to the average spacing of seeps along the drift, which is presumably related to quantities such as fracture and fault spacing, permeability distribution, and permeability correlation length. Data on these quantities are needed, but field data relating them to seep spacing are required in order to gain confidence in the model.

Even more so than for mountain-scale flow, seepage into drifts is potentially strongly affected by channeling of flow and discrete fracture effects. The adequacy of the current fracture continuum model to represent these effects must be examined, and the only real way to assess its adequacy is by testing it against field data. Testing of the model against observed seep spacing at analogue sites such as Rainier Mesa or Apache Leap could provide the needed coupling between fracture statistics and seep spacing. Additional niche tests should be conducted in all three repository hydrogeologic units (Topopah Spring Lower Lithophysal, Topopah Spring Lower Nonlithophysal, and Topopah Spring Middle Nonlithophysal, where the first niche test was conducted) in the east-west cross drift. The main ESF tunnel does not go through the Topopah Spring Lower Nonlithophysal, but the east-west cross drift is designed to go through all three hydrogeologic units of the repository.

A potentially important issue that was not addressed is the stability of seep locations over time. In the present models, seeps are assumed to occur at the same locations indefinitely, so that a fraction of the waste packages (the seepage fraction) is always wet and the rest are always dry. If seep locations changed with time, more waste packages would be contacted by seeps, but only for a fraction of the time. This effect could result in more waste packages failing, but over a longer period of time, which could be important for performance. Thus, the consequences of seep movement should be investigated.

Additional needs are assessments of the effects of episodic percolation pulses, the potential increase in seepage during drainage of thermally mobilized water, the effects of chemical or mechanical alterations in hydrologic properties around the drifts, and the effects of drift collapse or emplacement of backfill.

alpha at the top of the TSw unit. It was not used here because calibrations that used upstream weighting at those interfaces had already been performed.) The flow transitions back to the matrix within the Calico Hills unit, but it should be noted that the total downward flow is significantly reduced (nearly two orders of magnitude) in the lower portions of the model domain. This result is again consistent with the presence of perched water near the top of the Calico Hills, which apparently diverts flow laterally. Results of other base-case simulations at this location are similar.

Figure 2-101 shows the normalized fracture and matrix mass flow rates for simulation mnaqb_p (present-day infiltration, mean fracture alpha) along borehole SD-12. Because the presence of perched water is reduced in the location of SD-12, the total downward flow is attenuated less toward the bottom of SD-12 relative to SD-9. This further confirms that the presence of perched water in the northern part of the repository diverts a significant amount of flow laterally. Also, note that the downward flow at the bottom of SD-12 has transitioned into the matrix because there is vitric in Calico Hills.

Areal plots of total percolation flux (fracture plus matrix) using the expected base-case with LTA infiltration (mnaqbfl) are shown in Figure 2-102. The total percolation at the repository is nearly the same as the infiltration at the surface, confirming the primarily vertical flow between the surface and the repository as shown in Figure 2-92. However, significantly less percolation reaches the water table in the northern vicinity of the repository, where perched water was shown to divert flow laterally in Figure 2-92. Hence, Figure 2-102 shows large regions of "red" where perched water has diverted percolation. Regions of high percolation ("purple") appear where the diverted water eventually meets the water table, which is about 80 m higher than in the present-day infiltration simulations. Aside from the change in water table elevations, the general flow pattern is similar among the different climate scenarios.

2.5.1.3 Transport from Repository to Water Table

The aqueous travel time between the repository and the water table is also an important facet to performance. The groundwater-travel time can be assessed by tracking tracers from the repository to the water table. Five hundred thousand nonsorbing, nondiffusing particles are released from 360 elements that make up the repository (Figure 2-93) at time zero. Hydrodynamic dispersion was neglected (in the context of not including a physical-dispervisity value in the model). Figure 2-103 and Figure 2-104 show the cumulative breakthrough curves of this unretarded tracer at the water table for the base-case simulations.

Figure 2-103 shows that the infiltration rate, as dictated by the present-day, LTA, and superpluvial-climate conditions, has a significant influence on travel times between the repository and water table. While less than 25% of the particles reached the water table within 1,000 years in the present-day climate, nearly 95% of the particles reached the water table within 1,000 years in the superpluvial climate. The travel time of particles in the LTA climate fell in between those of the present-day and superpluvial climates. The arrival of particles at the water table was bi-modal because the model was of a dual-continuum nature. The earliest arriving particles (as indicated by the "knee" in the curves) were transmitted through the fracture continuum, while the later arriving particles were transmitted in the matrix. Nearly 30% of the tracer particles reached the water table via the fractures in the LTA and superpluvial cases, yielding a rapid travel time of less than 1 year.

Figure 2-104 shows the breakthrough curves for all five base-case simulations using the LTA climate scenario. The infiltration is seen to be the strongest driver for travel time and shape of the breakthrough curves. The variation in fracture alpha does not affect the breakthrough curves significantly for the unretarded tracer used in these analyses. However, sensitivity studies with matrix diffusion ~10^{-11} m^2/s show some sensitivity of the breakthrough curves to the various fracture alphas.

2.5.1.4 Guidance for Sensitivity Studies

Based on the foregoing results, it is evident that infiltration plays a dominant role in the resulting percolation fluxes and travel times beneath the repository. Therefore, additional simulations have been performed that investigate wider ranges of infiltration (times 5 and divided by 5). In addition, based on parameter sensitivity studies performed in Section 2.4.3.2.3, the calibration of additional property sets has been performed and is discussed in Section 2.6.1. Results indicate that increased infiltration directly increases percolation fluxes and decreases travel times beneath the repository. More details are given in Section 2.6.1.1.

2.5.2 Seepage

2.5.2.1 Percolation Values

As described in foregoing sections, the UZ-flow base case for TSPA-VA consists of fifteen site-scale flow fields, as listed in Table 2-37. However, the seepage base case was developed in parallel with development of the UZ-flow base case, and the initial determination of what percolation-flux range to use, etc., was made using an earlier version of the UZ flow, called the "preliminary base case," which is described further in Section 2.6.1.1.1. The preliminary-base-case flow fields are nearly the same as the base-case flow fields, except that a wider range of infiltration uncertainty was assumed—ranging from the base infiltration divided by five up to base infiltration multiplied by five rather than from base divided by three up to base times three. In addition, the preliminary base case did not include systematic variations of fracture alpha, so that there were only nine flow fields (three infiltrations times three climate states).

In order to run the seepage model for the appropriate range of percolation values, we looked at the distribution of percolation rates over the repository area for the nine preliminary-base-case flow fields produced by the site-scale model. Figure 2-105, Figure 2-106, and Figure 2-107 show histograms of the percolation flux at the repository for the three base-infiltration flow fields, which are denoted Qb, Qb_f1, and Qb_f2 (refer to Table 2-57). These figures show that percolation is quite variable over the repository. Summary statistics for the distributions shown, plus those for the other preliminary-base-case flow fields, are shown in Table 2-41 (refer to Table 2-57 for nomenclature). To conservatively capture the behavior at the high end of the flux range, we ran the seepage model for flux values at the 95th percentile level rather than mean values. The percolation values chosen for analysis are 14.6 mm/yr, 73.2 mm/yr, and 213.4 mm/yr. In addition, based on the results of those runs, 500 mm/yr was chosen as a fourth percolation value to analyze.

2.5.2.2 Fracture α and *k* Values

As already discussed, there are no actual measurements of fracture-hydrologic properties. All values that are used are based on conceptual models or analogs, and it is uncertain how well they represent the actual behavior of the UZ at Yucca Mountain. As discussed in Section 2.4.3.1.2, the conceptual model being used here to derive values for fracture α is based on the capillary-rise equation and measurements of air permeability and fracture density. For the three repository units—tsw34, tsw35, and tsw36 (the Topopah Spring Middle Nonlithophysal, Lower Lithophysal, and Lower Nonlithophysal, respectively)—the range of calculated α values is typically about an order of magnitude or so (see Section 2.4.2.1). Thus, we decided to use a range of one order of magnitude centered on the primary value. Specifically, the seepage model was run for α values of 3.3×10^{-4}, 9.7×10^{-4}, and 3.3×10^{-3} Pa^{-1}. The relative weights of the three values were set to 0.25, 0.5, and 0.25, respectively. This choice is somewhat arbitrary, but reflects a desire to allow significant probabilities for the outlying values, while giving the primary value preference.

The geostatistical heterogeneity model already includes spatial variability of fracture permeability, of course, but there is also a larger-scale component of the heterogeneity. For example, the borehole air-permeability tests typically indicate permeability values about an order of magnitude lower than those indicated by the pneumatic-calibration work (in TSw). One possible explanation for this discrepancy is that the higher pneumatic-calibration values represent the permeability of very large fractures and features that may have average spacing of tens of meters or more. Thus, they are not very representative of typical conditions at the drift scale and one does not want to base the drift-scale model on them. Even aside from the very-large-scale pneumatic-calibration permeabilities, there is significant variability in measured borehole air permeabilities. The standard deviation in log space is typically about 0.5 or so for TSw (see Section 2.4.3.1.2). Based on this, the seepage model is run with a range of two orders of magnitude in the mean fracture permeability, representing two standard deviations on either side of the primary value. The actual values used were 10^{-14}, 10^{-13}, and 10^{-12} m^2. When using the values other than the primary value, the same heterogeneity structure was used (depicted in Figure 2-55), with all permeability values simply scaled up or down by a factor of ten. The relative weights of the three values were set to 0.25, 0.5, and 0.25, respectively, with the same reasoning as above. The values used for the model runs and the relative weights are summarized in Table 2-42 (the sum of each row or column adds up to the weights given above).

It is important to note that we treat these ranges of values as uncertainty, not as spatial variability. Certainly there is both, but our conceptual model is that the combinations in Table 2-42 represent the uncertainty in the values, while spatial variability is represented by the geostatistical variations described in Section 2.4.4.2.1.

2.5.2.3 Model Results

The base-case seepage model (three-dimensional, heterogeneous fracture k, X_{fm}=0, steady state) was run for the matrix of cases shown in Table 2-42, for the four percolation rates listed above in Section 2.5.2.1. Each case was run for three geostatistical realizations (the three "parts" described in Section 2.4.3.2.1) in order to encompass more of the variability of the system. Thus, a total of $9 \times 4 \times 3 = 108$ three-dimensional simulations were run with TOUGH2. The results are tabulated in Table 2-43 through Table 2-53. For each combination of parameters, three seepage rates are given, for three 5-m drift segments, representing three waste-package-sized areas. Thus, the seepage rate represents the amount of water that could contact a waste package if it were placed there.

Some important points about the results are:

1. The numbers given are percentages of the percolation flux flowing in the top boundary over a 15-m-long area the width of the drift. Thus, the actual seep flow rate is given by the percentage listed (divided by 100), times the percolation rate q, times an area of 75 m^2, (15 m $\times$ 5 m).

2. The seepage percentages are given two ways: In Table 2-43a, Table 2-44a, etc. are given the seepage into the top half of the drift (from spring line to spring line). In Table 2-43b, Table 2-44b, etc. are given the total seepage into the drift. The difference is the amount that seeped into the bottom half of the drift, which happens sometimes if there is a low-permeability obstruction that channels water toward the lower part of the drift. The total seepages are given for information, but only the seepages into the top half of the drift are used for input to the rest of the TSPA. The reasoning for this is simply that water seeping in the side of he drift would not be able to drip onto a waste package.

3. A waste package is only about 1.5-m wide, but we are counting all seepage from a 5-m-wide area as potentially contacting a waste package. This choice should be conservative. It is intended to cover some effects that have not been explicitly included in our model such as drift collapse and backfill that could spread out an incoming plume.

2.5.2.4 Distributions for f_S and Q_S

From the tables of results in the previous section, project personnel derive appropriate distributions of seepage fraction (fraction of waste packages contacted by seeps, denoted by f_S) and seep flow rate (flow rate of water onto a waste package that is contacted by one or more seeps, denoted by Q_S), for use by the near-field, waste-package, and waste-form components of the TSPA. These distributions, which vary as functions of percolation flux, constitute the base-case abstracted seepage model for TSPA-VA.

To begin, Table 2-55 gives summary statistics for the distributions defined by the seepage rates in Table 2-43a through Table 2-53a combined with the weighting factors in Table 2-42. The distributions from which to sample f_S and Q_S by applying these statistical descriptors to beta probability distributions are defined. A beta distribution is uniquely specified by a minimum, a maximum, a mean, and a standard deviation. For f_S, the minimum and maximum are obviously 0 and 1. For Q_S, the minimum is again 0, but there is no obvious choice for the maximum. However, if the maximum is set to a large value, it will not affect the distribution significantly in the part of the distribution that is actually being sampled. That is, the maximum value will affect the shape of the distribution only far out on the tail, at probability values that are very unlikely to be sampled when 100 or 1,000 samples are drawn. Thus, we set the maximum value of the Q_S distribution to be 10 standard deviations above the mean.

An example of a beta-distribution fit to the calculational results is shown in Figure 2-108, which shows a cumulative distribution function (CDF) defined for f_S at q=73.2 mm/yr along with the beta distribution defined by the mean and standard deviation. Considering that there are only a few data points (one f_S value for each hydrologic-property set in Table 2-42—f_S is just the fraction of the drift segments that have some seepage), the beta distribution fits the CDF reasonably well.

Since we have results for only a few percolation fluxes, we must specify how to extend the distribution definitions to other fluxes. For percolations within the range of the calculational results, the simplest choice is to use linear interpolation between the points. Above the range, we extrapolate linearly. Fortunately, it is only for the superpluvial climate applied to the high-infiltration case (i.e., flow field Qbx5_f2) that percolations ever get that high. Below the calculational range (i.e., below 14.6 mm/yr), if the mean Q_S values are extrapolated linearly they go to zero at 7.2 mm/yr. The standard deviation of Q_S extrapolates to zero at 7.9 mm/yr. Thus, for the calculational model of seepage being used, and with the parameter values and weightings being used, there is a threshold for seepage into drifts at about 7 mm/yr. Since it does not make much difference, we opted to take the lower of the two numbers, 7.2 mm/yr, as the threshold for the initial abstracted model. Note that if the mean goes to zero the standard deviation must as well, because any Q_S values greater than zero would imply a mean greater than zero. Note also that if Q_S goes to zero, implying no flow into drifts, then f_S must go to zero as well.

It is important to consider, however, how the abstracted seepage model is used. For the engineered-barrier-system calculations, the repository is divided into six regions (see Figure 2-93). In each region, the average fracture flux at the repository is calculated and used in the abstracted seepage model to determine the fraction of waste packages affected in that region and the water-flow rates onto those waste packages. (Only the fracture flux is used because matrix flow is not expected to seep into drifts and because the process-based seepage calculations were made with a fracture-only model.) The seepage threshold mentioned above is problematic within this method, because even though the average flux in a region is lower than the threshold there may be locations within the region that have flux above the threshold (see Figure 2-105, for example, which has a mean percolation very near the threshold but which shows that some locations have fluxes much higher than the threshold and others are below the threshold).

To address this problem, we took histograms of fracture flux at the repository horizon for each of the six repository regions, for the three lowest-infiltration cases (Qbd5, Qbd5_f1, and Qb). The initial abstracted seepage model described above (mean and standard deviation taken from Table 2-55, with both going to zero at 7.2 mm/yr and linear interpolation between values) was applied to each percolation in the histogram and the resulting average and standard deviation of f_S and Q_S were calculated, along with the average q. The results are shown in Figure 2-109 and Figure 2-110. The figures show lines for the initial abstracted seepage-model quantities, which go to zero at 7.2 mm/yr. The values calculated from the percolation histograms are also shown, and it can be seen that they are close to the initial lines for fluxes above about 9 mm/yr, but deviate significantly at lower fluxes. We conclude from this that the model does not require a correction for the spatial variability of percolation flux except at the low end. To make this correction, we add three of the new points, which envelop the other points, to the abstracted model, including an adjusted threshold value of 2.2 mm/yr.

The points added to the initial model, both for low percolations and high percolations, are shown in Table 2-56 (note that when the mean f_S goes to one, its standard deviation must go to zero because any f_S values less than one would imply a mean of less than one). The means and standard deviations for the base-case abstracted seepage model are plotted in Figure 2-111 and Figure 2-112. Figure 2-113 and Figure 2-114 illustrate the ranges of the distributions as they vary with percolation flux. Of particular note is that the seepage-fraction distribution is very wide over much of the percolation range, reflecting the great variability of the seepage process.

2.5.2.5 Thermal Perturbations

Repository heating will have a significant effect on seepage, at least for a period of time. During the boiling period there will be little or no seepage into the emplacement drifts, and before and after the boiling period seepage may be enhanced because of condensate drainage (Nitao 1997a, pp. 1-8). In addition, there could be permanent changes to seepage because of accumulation of mineral precipitates above the drifts or because of collapse of the drifts.

The only one of these effects that is included in the TSPA-VA base case is the reduction of seepage during the boiling period (based on the results of Nitao 1997a, pp. 1-8), and it is included by reducing seepage to zero when the drift-wall temperature above a waste package is above the boiling temperature. The other effects are more difficult to model, but consideration of them is recommended to obtain a more defensible model. A possible abstraction for thermal-hydrologic effects of seepage is discussed in Chapter 3 (Section 3.6.5) of the Technical Basis Documents.

2.6 SENSITIVITY STUDIES

2.6.1 UZ Flow

Sensitivity analyses have been performed to complement the base-case model presented in Section 2.5.1. The bases for these alternative models have been discussed in Section 2.4.3.2 and are summarized here. From parameter-sensitivity results reported by Bodvarsson et al. (1997, Chapter 7) and from additional sensitivity studies presented in Section 2.4.3.2, the key UZ-flow parameters are the infiltration, the fracture-matrix connection-area reduction factor, and the fracture van Genuchten alpha parameter. Also potentially important are matrix and fracture permeabilities, and the fracture van Genuchten *m* parameter (plus, for transport and possibly for TH, the fracture porosity), but these parameters appear to be less important than the first three above. As a result, additional sensitivity studies have employed the following:

- A wider range of infiltration rates (times 5 and divided by 5) was examined using the LBNL site-scale UZ-flow model. Parameter sets were calibrated to these different infiltration rates, and the percolation rates and travel times were compared to the base case.

- A second alternative UZ-flow model, the DKM/Weeps model, was defined that is similar in behavior to the Weeps model, which was used in TSPA-1991 (Barnard et al. 1992, 4.31 through 4.53) and TSPA-1993 (Wilson et al. 1994, Chapter 15, pp. 1-70). Measured and inferred values for all matrix and fracture hydraulic properties were used, and the fracture/matrix reduction factor was set equal to upstream relative permeability (Ho 1997, pp. 401-410; Bodvarsson et al. 1997, Chapter 7). If the fit to matrix-saturation data was not sufficiently good with this simple choice, the X_{fm} value was scaled up or down globally to get a reasonable fit to the data. There are two aspects of the DKM/Weeps alternative model that provide useful insights into repository performance. First, the DKM/Weeps model has more fracture-dominated flow than the base case, including the nonwelded layers, so it shows whether repository performance is adversely affected by a much greater fast-flow component than exists in the base-case model. Second, having X_{fm} as a dynamical variable that depends on the flow, rather than as a fixed factor, could lead to differences in behavior when climate changes (and during the thermal period in thermohydrological models).

- The matrix permeabilities in the Calico Hills zeolitic units have been varied from the statistical mean. This parameter was thought to have a significant influence on travel times from the repository to the water table, so their values were increased and decreased by one standard deviation to determine the potential effects on UZ transport.

The following sections present more details on the development and results of the above sensitivity analyses.

2.6.1.1 Infiltration Sensitivity Study

In this section, a set of simulations using a wider range of infiltration rates than those used in the base case is presented. A description of the parameter calibration for these simulations is provided, and the results are compared to the base case.

2.6.1.1.1 Property sets for infiltration sensitivity study

The property sets that were calibrated for the current sensitivity study were actually created before the development of the base case described in Section 2.4.3.1.4 above and were intended for use in TSPA-VA calculations. As a result, they were deemed the "preliminary base case." The primary difference between the preliminary base case and the base-case property sets (Table 2-19 through Table 2-23) is in the treatment of the van Genuchten fracture alpha (air-entry) parameter. In the preliminary base case, these parameters were estimated using calibration, but in the base-case property set, these values were prescribed as described in Section 2.4.3.2.2 to limit the degrees of freedom during calibration. Because the values of fracture van Genuchten parameters prescribed in the base case were more realistic than the calibrated values of the preliminary base case (Section 2.4.3.2.2), the preliminary base case was used only as a sensitivity analysis. The development of all other parameters aside from the fracture van Genuchten alpha parameter is identical to the process described in Section 2.4.3.1.4 above for the base case.

Three property sets were calibrated using the present-day infiltration, the present-day infiltration divided by five, and the present-day infiltration multiplied by five. Together with the LTA and superpluvial climate scenarios for each present-day scenario, a total of nine simulations were run as shown in Table 2-57 and Figure 2-115. The preliminary base-case parameter sets used in this infiltration sensitivity study are shown in Table 2-58 through Table 2-60.

2.6.1.1.2 Results of Infiltration Sensitivity Study

The hydrologic behavior resulting from the parameter sets used in this sensitivity study are nearly identical to the base-case simulations for the same infiltration rates. The predicted ambient saturations generally match well with observed borehole saturations, and flow patterns are the same as those shown for the base case in Figure 2-102. The partitioning of flow also behaves similarly to the base case; nearly all of the water is carried in the fractures of welded units and in the matrix of the nonwelded units as indicated in Figure 2-100 and Figure 2-101.

Table 2-61 shows the average fracture-percolation fluxes over the six repository subregions for each of the nine sensitivity runs shown in Table 2-57. The percolation values for the present-day infiltration cases are identical between the base case and the sensitivity run. However, as expected, the percolation values for the high and low bounds of the infiltration sensitivity runs are greater and lower, respectively, than the bounds of the base case. The nearly vertical flow above the repository results in a nearly direct mapping of the surface infiltration to the percolation flux at the repository. As a result, the case with superpluvial infiltration rates times five has approximately five times greater percolation values than the base-case superpluvial values. The influence of these extreme percolation values on travel times between the repository and the water table is presented in Figure 2-116. A total of 500,000 unretarded particles (no matrix diffusion, no dispersion) were released as a pulse uniformly over each node within the six repository subregions shown in Figure 2-93. The median breakthrough time for the superpluvial-times-five case is approximately 20 years, whereas the median breakthrough time for the present-day-divided-by-five case is over 10,000 years. This range of travel times is similarly captured by the base-case simulations presented in Section 2.5.1.3, although to a slightly lesser extent. Therefore, because current studies of infiltration indicate that the maximum present-day infiltration should not exceed a factor of three times the current present-day infiltration values (Section 2.4.2.9), the times-five and divided-by-five cases examined in this sensitivity analysis were not used in TSPA-VA.

2.6.1.2 DKM/Weeps Alternative Model

As introduced earlier, the DKM/Weeps model yields more flow through fractures throughout the entire unsaturated system, most notably in the nonwelded units. A significant reduction in the fracture/matrix conductance allows more water to stay in the fractures without being imbibed into the matrix. The reduction factor, as described in Ho (1997, pp. 401-412), consists of the upstream relative permeability for liquid flow. To aid in the calibration of the model to matrix saturations, a global X_{fm} is also used as an additional fitting parameter.

Sensitivity analyses described in Section 2.4.3.2.3 provided sensible ranges for the most sensitive parameter (fracture permeability) in the DKM/Weeps model. All other hydrologic properties in the DKM/Weeps model are based on direct property measurements (e.g., saturated matrix permeability) or on parameters inferred from direct measurements (e.g., van Genuchten's alpha parameters for fractures calculated from fracture permeability and frequency data through the cubic law (Domenico and Schwartz

1990, pp. 86-87) and capillary theory) (Wu et al. 1998, pp. 32-33 and 43). A matrix of five runs that included uncertainty in present-day infiltration and fracture permeability was developed and is shown pictorially in Figure 2-117. Together with the LTA and superpluvial-climate scenarios for each present-day scenario, 15 runs were performed. Table 2-62 summarizes the runs and the nomenclature associated with each of the runs. The five parameter sets calibrated to the present-day infiltration scenarios using the DKM/Weeps model are shown in Table 2-63 through Table 2-67.

2.6.1.2.1 DKM/Weeps Results

The predicted liquid saturations at SD-9 and SD-12 are shown in Figure 2-118 and Figure 2-119, respectively. Because the DKM/Weeps matrix permeabilities were not calibrated, the slightly lower values that were measured cause the matrix liquid saturations to be higher than in the base case. The predicted saturations for the other DKM/Weeps simulations are similar. Nevertheless, the general match between the predicted matrix saturations and the observed borehole saturations is comparable.

Table 2-68 gives the mean fracture-percolation flux over each of the six repository subregions for nine representative cases of the DKM/Weeps runs (see Table 2-62 for nomenclature). Similar to the base case, the infiltration was found to be the most sensitive parameter in changing the magnitude of percolation over each of the repository subregions. The variation of the fracture permeability did not have a significant effect on the percolation values at the repository because, in both cases, the flow in the vicinity of the repository was predominantly in the fractures. As shown in Table 2- 68, the values of the percolations fluxes are quite similar to those of the base case.

The primary difference between these two models is in the partitioning of flow between fractures and matrix in the nonwelded units. Figure 2-120 through Figure 2-123 show the fracture- and matrix-percolation flux at the repository and at the water table for the DKM/Weeps run with mean present-day infiltration (kmnqb_p). The fracture- and matrix-percolation flux at the repository is nearly identical to that of the base case. However, there is an increased amount of flow in the fractures at the water table in the DKM/Weeps simulation as compared to the base case in particular regions (Figure 2-98 and Figure 2-122). The increased partitioning of flow in the fractures can be quantified in one-dimensional plots of fracture and matrix flow as a function of elevation along SD-9 and SD-12 (Figure 2-124 and Figure 2-125, respectively). The flow through the nonwelded PTn unit at SD-9 is almost entirely in the fractures using DKM/Weeps; in the base case, the flow is almost entirely in the matrix. Below the repository at SD-9, the total flow is greatly attenuated because of the presence of perched water. At SD-12, the flow through the nonwelded PTn unit is predominantly in the fractures using DKM/Weeps. This contrasts the predominantly matrix flow in the PTn unit at SD-12 for the base case. Below the repository at SD-12, the DKM/Weeps model yields a nearly equal partitioning of flow between the fractures and matrix in the Calico Hills unit. The base case resulted in predominantly matrix flow in the Calico Hills unit below the repository at SD-12. In some locations toward the center of the repository, the DKM/Weeps model yields predominantly fracture flow throughout the entire UZ.

Figure 2-126 shows tracers that were released as a pulse at two surface locations (10 particles at each location) above the left and right ends of the repository along two east-west vertical cross-sections (N235,000 and N233,400). The LTA infiltration scenario was used with the mean fracture permeability (kmnqbf1). The open symbols denote a higher concentration of the tracer in the fracture, while the solid symbols denote a higher concentration in the matrix. The movement of the unretarded tracers for the DKM/Weeps simulation is similar to that of the base case shown in Figure 2-92, but the partitioning of flow between fractures and matrix is different. In the PTn, the tracers are partitioned more in the fractures in both cross-sections than in the base-case simulations. Also, flow beneath the repository in the DKM/Weeps simulations shows more fracture flow, although the partitioning is not as pronounced as in the PTn unit. Lateral diversion caused by perched water still exists in the north cross-section, and flow patterns are very similar between the DKM/Weeps and base-case simulations.

The consequence of the increased fracture flow can be seen in Figure 2-127, where the breakthrough curves of a pulse of unretarded tracer released at the repository using the DKM/Weeps simulation (kmnqb) are presented. Compared to the results of the base case, the travel times are much shorter as a result of increased transport through fractures in the DKM/Weeps simulation. Nearly 50% of the tracer exhibits an early arrival (less than 1 year) via fractures during the superpluvial and LTA climates, and approximately 40% of the tracer experiences early arrival during the present-day climate. This has important consequences for repository performance during times less than 10,000 years. The fast transport of radionuclides through fractures using the DKM/Weeps model increases the dose rates at times less than 10,000 years when compared to the base case; however, for longer times (~100,000 years), the effect of rapid transport through fractures does not significantly impact the long-term dose.

The effects of varying fracture permeability on the DKM/Weeps model is shown in Figure 2-128. The breakthrough curves for all long-term-climate scenarios using the DKM/Weeps model are presented. Unlike the base case, the parameter variation has a significant effect on the travel time in addition to the infiltration variation. Runs with the maximum permeability (see Table 2-35 for range of fracture permeabilities used in DKM/Weeps simulations) show a significant amount of transport through the fractures. For the case using LTA infiltration multiplied by three (I*3) and a maximum fracture permeability, over 90% of the tracer arrives at the water table within 1 year. The same infiltration combined with a minimum fracture permeability results in 60% of the tracer arriving at the water table within 1 year. A similar disparity is observed in Figure 2-128 when the long-term-average infiltration is divided by a factor of three (I/3) and a range of fracture permeabilities is used.

The increased flow through the fractures also allows a fast component of flow between the surface and repository. As emphasized by the Performance Assessment Peer Review (PAPR) Panel, isotopic evidence (bomb pulse) indicates that travel times between the surface and some portions of the ESF can be less than 50 years (Fabryka-Martin et al. 1998, pp. 93-96). The exact disposition of these fast flow paths is unclear, but the existence of bomb pulse at the repository horizon appears to be more concentrated near faults. Figure 2-129 shows the paths of unretarded tracer released from the surface along a vertical east-west cross-section through the center of the repository (N233,400 m). The tracer was released as a pulse (100 particles at 5 surface locations), and the paths of the tracer during a 50-year period were recorded as indicated by the locations of the symbols in the plots. In the DKM/Weeps simulation, the tracer has reached the repository (shown as a solid line) at all locations. In the base-case simulation, the tracer only reaches the PTn unit in 50 years over most of the repository. Near the Solitario Canyon fault, which borders the west end of the repository, the tracer has propagated past the repository horizon in the base-case simulation. The observation of increased bomb pulse near faults is consistent with the predicted behavior of the base-case model, but the existence of bomb pulse in regions away from faults is not predicted by the base-case model. In contrast, the DKM/Weeps model predicts that fast paths can occur at all locations. It is important to note that Figure 2-129 does not indicate that all of the particles in the DKM/Weeps model have propagated past the repository horizon during the 50-year period. The figure just shows all locations where a particle has resided at any point in time.

2.6.1.3 Zeolitic Matrix Permeability

Additional flow fields were generated using the three-dimensional UZ site-scale model to evaluate the sensitivity of the model to the matrix permeabilities used for the zeolitic layers. The base-case simulation using LTA infiltration (mnaqbf1) was used as the reference case. Each model layer, including layers ch1zc, ch2zc, ch3zc, ch4zc, pp2zp and bf2zp, was altered by increasing and decreasing the existing matrix permeability of each layer by one standard deviation. Other rock properties were not re-calibrated with the modification of the zeolitic matrix permeabilities. The standard deviations used are the ones listed in Table 5.2.2 of Wu et al. 1998, pp. 24-26) and are also listed in Table 2-69 of this document. Steady-state hydrologic conditions were obtained using the EOS9 module of TOUGH2 as described in Section 2.4.3.9 for cases in which the zeolitic matrix permeability was increased and decreased by a standard deviation.

Figure 2-130 shows the breakthrough of a tracer at the water table released as a pulse (500,000 particles) uniformly over the repository for the base-case LTA simulation. Figure 2-130(a) shows the results for an unretarded tracer (no matrix diffusion, no sorption), while Figure 2-130(b) shows the results for a tracer with a sorption coefficient (Kd) of 2.5 cc/g in the zeolitic-matrix units. For the simulations with an increased zeolitic-matrix permeability, the breakthrough curve exhibits longer travel times. The increased zeolitic-matrix permeability allowed more flow to occur through the matrix (note the slightly lower fraction of particles that arrive at early times through fractures); thus, more particles were transported (at slower rates) through the matrix. The delay associated with increased zeolitic-matrix permeabilities is most notable when sorption occurs in the zeolitic-matrix as shown in Figure 2-130(b). Decreasing the zeolitic matrix permeability did not change the breakthrough curves significantly. A decrease in the zeolitic matrix permeability causes more flow to be diverted in the zeolitic fractures (yielding shorter travel times), but because the partitioning of flow was already predominantly in the fractures, the impact of decreasing the zeolitic-matrix permeabilities was small.

2.6.2 Seepage

Three sensitivity analyses were conducted in which the weightings in Table 2-42 were modified. Two kinds of modifications to the seepage-model inputs are made. One is to narrow the fracture-property distributions (i.e., assume that the fracture properties have less uncertainty than in the base case) and the other is to skew the distributions toward higher or lower fracture apertures.

As discussed previously, three values of fracture permeability (k_f) and three values of fracture alpha (α_f) were used in the drift-scale flow simulations that were performed to calculate the amount of seepage into emplacement drifts. The base-case weights for both parameters were assigned as (0.25, 0.5, 0.25); that is, the lowest value was weighted 25%, the middle value 50%, and the highest value 25%. The middle value is the preferred value, based on the available data, and the low and high values were chosen to span a reasonable range based on the variability in the data. For the first sensitivity analysis, the weights of the outlying values were cut in half, giving weights of (0.125, 0.75, 0.125). These weights emphasize the best-estimate parameter values considerably more. They are also reasonable, given what is known about fracture properties. Taking fracture permeability as an example, the base-case weights imply a log standard deviation (i.e., the standard deviation of the logarithm of permeability) of 0.7, while the narrower distribution implies a log standard deviation of 0.5. These standard deviations are near the low and high ends of the observed range for air-permeability measurements in the repository host rock (see Table 7.11 of Bodvarsson et al. 1997).

This modified set of weights was applied to the process-model results to generate new seepage distributions, and then TSPA calculations were run with the modified seepage distributions. The modified statistics for f_s and Q_s are shown in Figure 2-131 and Figure 2-132.

The other two sensitivity analyses have modified weights that represent systematically smaller or larger fractures. These cases could approximate the possibility of smaller or larger fracture apertures caused by thermal-hydrologic-chemical or thermal-hydrologic-mechanical processes. Smaller fracture apertures imply both lower k_f and lower α_f, because α_f is proportional to the effective fracture aperture and k_f is proportional to the cube of fracture aperture. Therefore, to simulate smaller fracture apertures, the weights for the parameter values were shifted to smaller values, giving (0.67, 0.33, 0) as the low, middle, and high parameter values. Similarly, to simulate larger fracture apertures the weights were changed to (0, 0.33, and 0.67). The resulting seepage parameters are plotted in Figure 2-133 through Figure 2-136.

2.7 SUMMARY AND RECOMMENDATIONS

This chapter has detailed the development of four major components of UZ flow: (1) climate, (2) infiltration, (3) mountain-scale UZ flow, and (4) drift-scale seepage. Issues associated with each component have been presented, along with abstraction/testing plans that addressed these issues. The bases for the development of climate and infiltration models, UZ flow models, and seepage models were discussed, along with a number of sensitivity analyses to investigate relevant processes and parameters. Results for the base-case UZ flow and seepage simulations were then presented, and a series of sensitivity analyses were also discussed. The following sections summarize each of the four major UZ-flow components. The impact of each component on performance, along with guidance and recommendations for license application, are also provided.

2.7.1 Climate

The primary purpose of climate modeling was to provide precipitation rates and water table elevations that varied as a function of future climates. Future climate was modeled in TSPA-VA as a sequence of discrete steady states. Only three discrete climate states were considered for TSPA-VA: present-day, LTA, and superpluvial. Present climate represented relatively dry, interglacial conditions, while the LTA represented an average pluvial period at Yucca Mountain. The superpluvial represented periods of extreme wetness. The MAP for the present, LTA, and superpluvial climates were estimated to be 150, 300, and 450 mm/yr, respectively, as shown in Table 2-5. These values were used by infiltration modelers to determine appropriate analog sites that had average precipitation rates that were commensurate with the predicted future climate values. The water-table rise from the present-day level (~730 m) was estimated to be 80 m and 120 m for the LTA and superpluvial climates, respectively. The duration of each cycle is tabulated in Table 2-7, but sensitivity analyses have shown that the overall performance is not sensitive to the duration of the climate cycles. The most significant impact was found to be the abrupt changes in water-table elevation and groundwater flow rate that occurred at the transition between climates. Section 2.4.1 provides more details of the climate modeling, and additional information on the development of the climate models can be found in CRWMS M&O (1998, Section 4).

2.7.1.1 Implications for Performance

Climate models strongly impact performance through their influence on precipitation and evapotranspiration. These factors, in turn, influence the predicted infiltration in the UZ-flow model. Therefore, the magnitude and timing of the prescribed climate states is important to performance.

2.7.1.2 Guidance for License Application

Additional work is needed to understand the natural variability of current and future climates for Yucca Mountain. In particular, the adequacy of three distinct climate states needs to be addressed further. If distinct climate states are used in future analyses, their number, timing, duration, and the abruptness of the transition between them need better support. Additional modeling is needed to determine how the dose-rate pulses depend on the time of transition between climates, and whether noninstantaneous transitions would lead to lower peak doses. Appropriate climate analogs need to be defined, based on temperature and other factors in addition to precipitation. The superpluvial climate, especially, needs better definition.

2.7.2 Infiltration

Infiltration modeling provides the spatial and temporal distribution of net infiltration as an upper boundary for site-scale UZ-flow models in TSPA-VA. Distributed net infiltration rates were determined for each of the three climate states using the YMP infiltration model described in Section 2.4.2 (also presented in CRWMS M&O 1998, Section 5.3.4.1). The infiltration model simulated water movement at the ground surface by solving water mass balances using precipitation, a model for evapotranspiration, and available water in the soil profile. Also considered in the model were ground surface elevation, slope, bedrock geology, soil type, soil depth, and geomorphology. The primary driver for the infiltration model was precipitation, which was input using available records or, in some cases, a stochastic model. Daily precipitation records from different locations were used to define the present-day, LTA, and superpluvial climates in the infiltration model. The sites were chosen based on how well their MAP values matched the estimated values associated with each climate. Table 2-10 summarizes the location of the analog sites and the measured and predicted values of precipitation. General results of the infiltration model are as follows:

- The modeled infiltration is highly heterogeneous and clearly correlated with topographic features
- The highest net infiltration occurs along Yucca Crest
- Net infiltration is lower in washes.

The spatially distributed infiltration maps were then upscaled to the site-scale UZ-flow model by averaging the simulated infiltration values over each surface element in the UZ-flow model. Figure 2-18, Figure 2-19, and Figure 2-20 show the infiltration maps for the present-day, LTA, and superpluvial climate scenarios. The average infiltration for each climate over the UZ-flow model domain are 4.9, 32.5, and 118 mm/yr, respectively.

Sensitivity analyses were also conducted to determine the effects of episodic infiltration on the percolation at the repository horizon (Section 2.4.2.8). Results showed that the PTn unit effectively damped episodic pulses that were simulated on a yearly cycle, preventing the transient pulses from significantly impacting the percolation at the repository horizon.

Additional sensitivities that used infiltration to estimate the temperature profile in a borehole indicated that infiltration rates that were greater than three times the average present-day infiltration rate did not allow good matches with observed borehole temperatures because of increased advective heat transfer. Therefore, a factor of three was used as the upper and lower bounds for the range of infiltrations considered in each climate scenario (see Figure 2-52).

2.7.2.1 Implications for Performance

Infiltration strongly influences repository performance because of its influence on mountain-scale unsaturated-zone flow and seepage into drifts (which subsequently affects waste-package-degradation models). The infiltration rates used in TSPA-VA are significantly higher than in past TSPAs. Higher infiltration rates, in general, tend to adversely impact total performance. However, the increased infiltration must be considered in conjunction with other TSPA components such as seepage to understand the overall impact on performance.

2.7.2.2 Guidance for License Application

The greatest need for improvement is explicit inclusion of processes that should be different for future climates, including effects of temperature, cloudiness, vegetation type, surface water runoff/run-on, and snow cover. Even for current conditions, some experts in the UZFEE (CRWMS M&O 1997) suggested that runoff and run-on might be more important than is assumed in the infiltration model.

To provide a more quantitative basis for the uncertainty distribution for infiltration, the infiltration model should be run in a stochastic mode (e.g., Monte Carlo simulation) to derive the infiltration uncertainty from the uncertainties in the input parameters of the model.

Finally, analogues with known infiltration, such as Rainier Mesa and Apache Leap, should be used to test and improve the infiltration models and methods.

2.7.3 Unsaturated Zone Flow

The three-dimensional LBNL UZ-flow model has been used to calculate unsaturated-groundwater flow at Yucca Mountain for TSPA-VA. The model implements the dual-permeability formulation for fracture-matrix interactions and consists of nearly 80,000 elements. Hydrologic properties were determined using both direct measurements and calibration with field data (Section 2.4.3.1), which included core samples, borehole log data, in situ water potential and temperature measurements, fracture measurements from the ESF, in situ pneumatic data, air permeability tests, and geochemistry data. A great deal of information on the calibration and details of the LBNL UZ-flow model development was taken from Bodvarsson et al. (1997, Chapters 1-4, 6-8, 10-11, 13, 15, 17-19). In the calibration approach, a number of vertical one dimensional submodels that corresponded to borehole locations were extracted from the three-dimensional model. The code ITOUGH2 was used to perform simultaneous inverse simulations with these one-dimensional models to optimize hydrologic parameters by matching predicted and observed matrix saturations and moisture potentials. The selection of hydrologic parameters that were estimated by inverse modeling were influenced by sensitivity studies (Section 2.4.3.2) that determined important parameters to UZ flow, which included the fracture air-entry parameter, α_f, and the fracture-matrix interaction parameter, X_{fm}. The properties that were calibrated in one dimension were then used in the three-dimensional site-scale model, which included calibrations to perched water. Figure 2-52 shows a tree-diagram of the resulting parameter sets that were used for the base case in TSPA-VA, and Table 2-19 through Table 2-24 show the resulting property values for all materials. Additional tests using geochemical data, infiltration data, and alternative weighting schemes were also performed to improve the three-dimensional model and increase confidence in the methods being used (Section 2.4.3.5 and Section 2.4.3.6).

Results presented in Section 2.5.1 show that the flow through the UZ is predominantly in the fractures for the welded units and predominantly in the matrix for the nonwelded units. High infiltrations resulting from climate changes significantly increased the percolation flux in the vicinity of the repository and decreased the travel time between the repository and the water table. Travel times between the repository and the water table ranged from several days to hundreds of thousands of years (Figure 2-103). The fastest transit times resulted from flow through fractures, whereas the matrix contributed to particle breakthrough at the water table at significantly longer times. Perched water, which has been calibrated in the three-dimensional flow model, diverted vertical flow laterally in the three-dimensional model, especially in the northern part of the repository (Figure 2-92). However, the total travel time of the diverted water was not significantly altered due to the fast flow path through the fractures. Sensitivity results using increased infiltration confirmed the importance of infiltration rates in determining travel times between the repository and the water table. In addition, sensitivity results using the DKM/Weeps alternative model showed that there was more significant fracture flow than in the base case, contributing to faster travel times. Finally, sensitivity studies of the zeolitic matrix permeability showed that increased matrix permeability can result in slower travel times due to increased flow through the matrix. However, decreased matrix permeabilities did not result in significant changes from the base case.

2.7.3.1 Implications for Performance

A significant result of the current TSPA-VA UZ flow calculations relative to earlier TSPAs is that the higher estimates of current and future infiltrations can cause percolation fluxes to be significantly greater and travel times to be significantly shorter. While these effects have a negative impact on performance, the impact of UZ flow in general on the total-systems performance calculations must be determined collectively with other system components. For example, high infiltrations are thought to be adverse to performance, but performance calculations have shown that for a period of time, the high infiltration scenarios show a decrease in dose for a period of time. This counter-intuitive result occurs because the temperatures around the waste package are reduced by the increased infiltration, and the corrosion of the waste packages is reduced.

The use of the DKM/Weeps model produced significantly shorter travel times between the repository and water table because of increased partioning of flow through fractures. As demonstrated in total-systems PA calculations, the decreased travel times increase dose rates for periods less than 10,000 years, but for longer times (100,000 and 1,000,000 years), the rapid transport does not significantly impact performance. At these later times, the travel time becomes small relative to the total simulation time, and the decreased travel time in the DKM/Weeps model is less important. However, colloid-facilitated transport can be enhanced by increased flow and partitioning in fractures.

The uncertainty in matrix permeability in the zeolitic units resulted in travel times that could differ by several thousand years. Sorbing tracers traveling through the zeolitic matrix were retarded more if the permeability was increased, but little difference was observed if the permeability was decreased. Because the matrix permeabilities in low-permeability units is likely to be less than the reported values because of excluded "nondetect" values, the uncertainty associated with matrix permeabilities may not significantly impact overall performance.

2.7.3.2 Guidance for License Application

The most important need in the mountain-scale, UZ flow modeling is a better representation of localized channeling of flow, and in particular, the effects of flow in discrete fractures. Current modeling uses continuum models with very coarse spatial discretization, and the adequacy of this approach is not fully established. There are indications from geochemical and isotopic tracers (chloride concentration, ^{36}Cl-to-chlorine ratio and ^{14}C-to-carbon ratio) that channeling of flow might be important. In addition, geochemical, isotopic, and temperature data should be integrated into the calibration procedure because they provide important information about flow through fractures.

More information is needed about the role of perched water in UZ flow. The current model assumes that the water is perched on a very-low-permeability underlying layer and flow is forced to go around it. Other interpretations are possible, such as mixing within the perched water and matrix flow out the bottom.

Thermal alterations of flow and TH-chemical or TH-mechanical alterations of hydrologic properties are potentially important. In the current TSPA structure, these effects fall under the TH component, but it is necessary to determine whether there should be a coupling of TH effects on mountain-scale, UZ flow and transport.

Technical recommendations for improvement of the current mountain-scale, UZ-flow model include the following:

- Incorporation of the most recent version of the integrated site model (site geologic framework model)
- More refined numerical grid
- Additional data to gain better estimates of fracture-hydrologic parameters
- Additional imbibition tests of hydrologic properties of the matrix
- Additional measurements of permeability of the zeolitic hydrogeologic units and properties of faults
- Additional studies to better characterize and understand the effects of perched-water bodies
- Creation of heterogeneous property sets that take advantage of the heterogeneous distributions provided by Rautman and McKenna (1997, pp. 1-322) and a stochastic representation of the parameter fields in the site-scale UZ model.

Fracture-flow processes should be further investigated with alternative conceptual models and additional field studies, such as niche and alcove studies, the planned east-west cross drift, and the Busted Butte transport study. Other flow processes that need to be further characterized include flow through faults, flow between disparate units (such as at the Paintbrush nonwelded–Topopah Spring welded and Calico Hills vitric–Calico Hills zeolitic interfaces), and fracture/ matrix interactions. Finally, the process of model calibration can be further improved by developing two-dimensional and three-dimensional calibrations against field data, which may require using parallel computing techniques.

2.7.4 Seepage

The abstracted base-case seepage model was based on a large number of three-dimensional process-model calculations. The process model consisted of a three-dimensional heterogeneous fracture-continuum field presented in Figure 2-55. Three blocks of dimensions 20-m high, 15-m wide and 16.5-m long were evaluated independently within this continuum. The drift was represented by a horizontal open cylinder of diameter 5 m at the center of the lower part of the block (Figure 2-56). Simulation grid cells were defined to be $0.5 \times 0.5 \times 0.5$ m. Fracture properties were obtained from air-permeability tests of the DST in the ESF Thermal Test Alcove 5 and from evaluation of fracture surveys in the ESF. As a conservative estimate, matrix flow was neglected in seepage simulations used for TSPA-VA, and sensitivity studies were performed to evaluate the effects of fracture-matrix interactions. Sensitivity studies were also performed to determine the effects of episodic pulses, variations to hydrologic properties, and grid refinement (Sections 2.4.4.5 through 2.4.4.8).

The process-model results were abstracted by fitting the calculated seepage-fraction (f_S) and seep-flow-rate (Q_S) distributions with beta probability distributions for which the mean and standard deviation are functions of percolation flux in the fractures (also, the maximum in the case of Q_S). The final abstracted models are illustrated in Figures 2-111 through 2-114. The seepage process model has been tested against recent preliminary data from the ESF niche liquid-release tests, and appears to fit them reasonably well. Finally, seepage sensitivity studies were performed to investigate reduced variance of fracture properties and variations to the fracture aperture. Results of the sensitivity are shown in Figure 2-131 through Figure 2-136.

2.7.4.1 Implications for Performance

Seepage into the drifts has a significant impact on performance for several reasons. Seepage controls waste-package degradation because the waste-package material (C-22) corrodes only in the presence of liquid water. Following the creation of openings through the C-22, the seepage volume controls the amount of water that can enter the waste package and dissolve the waste form. The flux of water into and through the waste package in turn controls the release rate of the solubility-limited radionuclides from the waste package. The impact of seepage on overall performance has been found to be important for periods ranging from 10,000 years to 1 million years.

2.7.4.2 Guidance for License Application

A number of additional studies have been identified that can be addressed in the near future (or are already underway) that will produce realistic and useful results for TSPA. They are listed below:

- One of the key factors that control the spacing between drip seepage locations is the correlation lengths of spatial heterogeneity of the rock unit. A further careful study of the fracture distribution along the ESF (Bodvarsson et al. 1997, Chapter 7) should be made to provide estimates of these parameters. Field data from the ESF niche study can also yield important information related to this factor.

- A more comprehensive parameter-sensitivity study should be made, including sensitivity of drift seepage to the width of the permeability probability distribution function and the spatial correlation lengths of the heterogeneous fields. The occurrence of special features, such as long fractures intercepting the drift, should also be studied. The range of situations and property values used should be representative of the three stratigraphic units in which the potential repository will reside.

- For reliable results, the study needs to be performed with more realizations in the sense of a stochastic analysis and with potentially finer grids. Previous sensitivity studies have indicated that seepage may increase with finer grids.

- Gravity-driven flux in near-field discrete fractures close to the drift wall may increase the probability of drift seepage. Additional study of this possibility is needed.

- Further study on successive percolation pulses should be carried out, especially since the current calculations seem to indicate that the time frame for the system to recover to its original initial state after the first pulse is very long, perhaps as long as hundreds of years.

The ESF niche test is an important first step in verifying seepage models, but it is primarily a test of the overall conceptual model of the drift opening acting as a capillary barrier. The test offers little validation of the calculated values of seepage fraction, which the TSPA results show to be the most important aspect of seepage—indeed, the most important aspect of repository performance. Seepage fraction, or the fraction of waste packages contacted by seepage water, is related to the average spacing of seeps along the drift, which is presumably related to quantities such as fracture and fault spacing, permeability distribution, and permeability correlation length. Data on these quantities are needed, but field data relating them to seep spacing are required in order to gain confidence in the model.

Even more so than for mountain-scale flow, seepage into drifts is potentially strongly affected by channeling of flow and discrete fracture effects. The adequacy of the current fracture continuum model to represent these effects must be examined, and the only real way to assess its adequacy is by testing it against field data. Testing of the model against observed seep spacing at analogue sites such as Rainier Mesa or Apache Leap could provide the needed coupling between fracture statistics and seep spacing. Additional niche tests should be conducted in all three repository hydrogeologic units (Topopah Spring Lower Lithophysal, Topopah Spring Lower Nonlithophysal, and Topopah Spring Middle Nonlithophysal, where the first niche test was conducted) in the east-west cross drift. The main ESF tunnel does not go through the Topopah Spring Lower Nonlithophysal, but the east-west cross drift is designed to go through all three hydrogeologic units of the repository.

A potentially important issue that was not addressed is the stability of seep locations over time. In the present models, seeps are assumed to occur at the same locations indefinitely, so that a fraction of the waste packages (the seepage fraction) is always wet and the rest are always dry. If seep locations changed with time, more waste packages would be contacted by seeps, but only for a fraction of the time. This effect could result in more waste packages failing, but over a longer period of time, which could be important for performance. Thus, the consequences of seep movement should be investigated.

Additional needs are assessments of the effects of episodic percolation pulses, the potential increase in seepage during drainage of thermally mobilized water, the effects of chemical or mechanical alterations in hydrologic properties around the drifts, and the effects of drift collapse or emplacement of backfill.

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