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Capillary Barriers in Unsaturated Fractured Rocks of Yucca Mountain, Nevada

For Submission to *Water Resources Research*

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ABSTRACT

This work presents modeling studies investigating the effects of capillary barriers on fluid-flow and tracer-transport processes in the unsaturated zone of Yucca Mountain, Nevada, a potential site for storing high-level radioactive waste. These studies are designed to identify factors controlling the formation of capillary barriers and to estimate their effects on the extent of possible large-scale lateral flow in unsaturated fracture rocks. The modeling approach is based on a continuum formulation of coupled multiphase fluid and tracer transport through fractured porous rock. Flow processes in fractured porous rock are described using a dual-continuum concept. In addition, approximate analytical solutions are developed and used for assessing capillary-barrier effects in fractured rocks. This study indicates that under the current hydrogeologic conceptualization of Yucca Mountain, strong capillary-barrier effects exist for significantly diverting moisture flow.

Key Words: Unsaturated zone, capillary barriers, lateral flow, unsaturated flow simulation, and fracture-matrix interactions.

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1. INTRODUCTION

It has long been recognized that capillary barriers may form under unsaturated conditions in layered, porous soils and formations [e.g., *Miyazaki*, 1988; *Ross*, 1990]. Capillary barriers may also form under unsaturated conditions in layered, fractured rocks [*Montazer and Wilson*, 1984]. Studies of the latter have been part of the unsaturated-zone (UZ) flow and transport site characterization efforts within the fractured tuffs at Yucca Mountain, Nevada. Located in the arid western United States, the thick unsaturated zone at Yucca Mountain is currently under consideration by the U.S. Department of Energy as a potential repository site for the storage of high-level radioactive waste.

The natural capillary-barrier concept has been of considerable interest in assessing the performance of the potential repository. Capillary barriers can potentially shield subsurface regions from downward percolation and reduce the potential for radionuclide mobilization and transport by advection. Capillary barriers may also retard the rate of percolation, leading to longer groundwater travel times. *Montazer and Wilson* [1984] were among the first to discuss the capillary-barrier concept. They hypothesized that capillary barriers exist at layer contacts where a unit with relatively small (fine) pores or fractures overlies a unit with relatively large (coarse) pores or fractures. More recent studies include estimation of lateral diversion capacity using an analytical approach [*Wilson*, 1996] and numerical modeling using a layered, porous medium model [*Moyer et al.*, 1996].

Quantitative analysis of capillary barriers and lateral flow has been performed using analytical approaches [*Ross*, 1990; *Warrick et al.*, 1997; *Webb*, 1997; *Morel-Seytoux et al.*, 1996; *Morel-Seytoux and Nimmo*, 1999] as well as numerical methods [*Rulon et al.*, 1986; *Oldenburg and Pruess*, 1993; *Pan et al.*, 1997; *Ho and Webb*, 1998]. Most investigations have focused on capillary barriers created by contrast in hydraulic properties of adjacent fine and coarse layers of homogeneous soils. *Oldenburg and Pruess* [1993] present modeling sensitivity analyses of mobility weighting schemes and spatial discretization, while numerical studies by *Pan et al.* [1997] investigate transient flow behavior. A recent study by *Ho and Webb* [1998] discusses the effects of heterogeneity within porous materials on capillary-barrier performance.

Despite the progress made in the general understanding of capillary barriers in porous soils over the last several decades, very few studies have been conducted and reported in the literature regarding the capillary-barrier phenomenon in fractured rocks. As a result, our understanding of capillary-barrier effects in unsaturated fractured rocks is currently limited. During early site characterization of the UZ at Yucca Mountain, the capillary-barrier and lateral flow concept was proposed and studied conceptually [*Montazer and Wilson*, 1984]. Subsequent numerical modeling investigations [*Rulon et al.*, 1986; *Wittwer et al.*, 1995; *Moyer et al.*, 1996; *Wu et al.*, 1998; *Wu et al.*, 1999] have shown a wide range of variability in the amount of lateral flow associated with capillary-barrier or permeability-barrier effects in fractured tuffs. Consequently, a general need has arisen for in-depth analyses or studies regarding the fundamentals of capillary barriers in fractured media.

Many types of data have been collected from the Yucca Mountain site over the past two decades. These data have been used to formulate a conceptual understanding of the mountain's hydrologic system. Based on this conceptual understanding, we have developed a comprehensive, three-

dimensional, unsaturated-zone (UZ) flow model for characterizing the unsaturated system [Wu *et al.*, 2000; Bodvarsson *et al.*, 2000]. Continual data collection and analyses have led to improvements in this quantitative predictive model of UZ flow and transport behavior at Yucca Mountain. The model provides an opportunity to test different conceptual ideas and to explore flow phenomena (such as capillary-barrier formation and lateral diversion) under the current ambient flow condition.

The systematic modeling study presented in this paper investigates the capillary-barrier phenomenon in fractured rocks using five two-dimensional (2-D), vertical cross-sectional models constructed using site-specific data from Yucca Mountain. The modeling approach is based on a dual-continuum, i.e., dual-permeability conceptual model, for handling fracture and matrix flow and interaction. The objectives of this work are to demonstrate: (1) whether an effective capillary barrier could develop at Yucca Mountain, and (2) what the controlling factors are for such a capillary barrier to form at the site. The 2-D modeling results show that effective capillary barriers are primarily determined by a combination of both matrix and fracture capillary gradients. Under the current hydrogeologic conceptualization of Yucca Mountain, strong capillary-barrier effects exist for significantly diverting moisture flow through a relatively shallow unit (the Paintbrush nonwelded unit). Major faults observed at the site are believed to serve as major downward pathways for laterally diverted percolation fluxes. In addition, we develop a simple analytical approach by extending the analytical solutions for flow through layered single-porosity soils using an effective continuum model (ECM).

2. HYDROGEOLOGIC SETTING AND CONCEPTUAL MODEL

As shown in Figure 2.1, the areal domain of the UZ model encompasses approximately 40 km² of the Yucca Mountain area [Hinds and Pan, 2000; Wu *et al.*, 2000]. Vertically, the UZ is between 500 and 700 m thick, and overlies a relatively flat water table in the vicinity of the potential repository area. The potential repository would be located in the highly fractured Topopah Spring Tuff, approximately 200 m or more above the water table.

Subsurface hydrologic processes in the UZ occur in a heterogeneous environment of layered, anisotropic, fractured volcanic rocks [Scott and Bonk, 1984]. These volcanic rocks consist of alternating layers of welded and nonwelded ash-flow and air-fall tuffs. From the land surface to the water table, the primary geologic units found at Yucca Mountain are as follows: the Tiva Canyon, Yucca Mountain, Pah Canyon, and Topopah Spring Tuffs of the Paintbrush Group, the Calico Hills Formation, and the Prow Pass, Bullfrog, and Tram Tuffs of the Crater Flat Group [Buesch *et al.*, 1995].

The major units within the UZ have been reorganized into major hydrogeologic units based roughly on the degree of welding within each unit [Montazer and Wilson, 1984]. These are: the Tiva Canyon welded (TCw) unit; the Paintbrush nonwelded (PTn) unit, consisting primarily of the Yucca Mountain and Pah Canyon Tuffs and their bedded tuffs; the Topopah Spring welded (TSw) unit; the Calico Hills nonwelded (CHn) unit; and the Crater Flat undifferentiated (CFu) unit. These major hydrogeologic units vary significantly in thickness over the model domain.

FIGURE 2.1 Plan view of the UZ model domain, showing the model boundary, the potential repository outline, major fault locations from GFM 3.1, the paths of the ESF and ECRB, selected boreholes, and the location of cross sections used in the capillary-barrier modeling studies described in this paper.

The hydrogeologic layering scheme used in this study is based on that of the current UZ flow model [Hinds and Pan, 2000], which is in turn based on the current Geologic Framework Model of Yucca Mountain (GFM 3.1) by Clayton [2000] and the analyses of rock properties data by Flint [1998]. In this geological model, the UZ of Yucca Mountain is represented by a stack of three-dimensional layers, each with its own set of fracture and matrix properties. In addition, these layers are intersected by several major faults (as defined in GFM 3.1). Table 2.1 correlates major and detailed geologic units with major and detailed hydrogeologic units and UZ model grid layers in the upper part of the unsaturated zone at Yucca Mountain, the focus of this study.

TABLE 2.1 Major hydrogeologic unit, geologic unit, UZ model layer, and detailed hydrogeologic unit correlation used in the PTn flow studies.

Major Hydrogeologic Unit	Geologic Unit		UZ Model Layer	Detailed Hydrogeologic Unit [Flint, 1998]
Tiva Canyon welded (TCw)	Tiva Canyon Tuff	Tpcr	tcw11	CCR, CUC
		Tpcp	tcw12	CUL, CW
		Tpcpv3	tcw13	CMW
		Tpcpv2		
Paintbrush nonwelded (PTn)	Tpcpv1	ptn21	CNW	
	Bedded tuff	Tpbt4	ptn22	BT4
	Yucca Mountain Tuff			
		ptn23	TPY	
		ptn24	BT3	
	Bedded tuff	Tpbt3	ptn25	TPP
	Pah Canyon Tuff	Tpp		
	Bedded tuff	Tpbt2		
	Topopa Spring Tuff	Tptrv3		
Tptrv2		ptn26	BT2	

Figures 2.2 through 2.5 display vertical geologic cross sections along transects identified in Figure 2.1. These cross sections focus on TCw and PTn units, though portions of the upper TSw appear in the lower parts of the figures. Figures 2.2 and 2.3 are east-west cross sections through the northern part of the potential repository area, along A-A' and B-B', respectively, in Figure 2.1. Transect A-A' has a lateral scale of one thousand meters (1000 m scale), while transect B-B' has a lateral scale on the order of four thousand meters (UZ model scale). Figure 2.4 is a north-south (N-S) cross section of the model domain through the potential repository area. Figure 2.5 is another east-west cross section (along transect C-C'), located in the southern part of the repository domain.

The PTn unit primarily consists of non- to partially welded tuffs and extends from the base of the densely to moderately welded, crystal-poor vitric subzones of the Tiva Canyon Tuff to the top of the densely welded, crystal-rich vitric subzone of the TSw. Thus, the PTn encompasses the nonwelded, crystal-poor vitric subzone of the lower Tiva Canyon Tuff, the pre-Tiva Canyon Tuff bedded tuff, the Yucca Mountain Tuff, the pre-Yucca Mountain Tuff bedded tuff, the Pah Canyon

Tuff, the pre-Pah Canyon Tuff bedded tuff, and the non- to partially and moderately welded, crystal-rich vitric zone subzones of the upper Topopah Spring Tuff. The dip of these layers is generally to the east at about ten degrees or lower.

Within the PTn, several layers (Tpcpv1, Tpbt4, Tpbt2, Tptrv3, and Tptrv2) are each less than 10 m thick within the potential repository footprint, while layers Tpy, Tpbt3, and Tpp show considerable variation in thickness across the potential repository area, with each showing a thinning trend to the south (Figures 2.4 and 2.5). The combined thickness of the PTn layers exceeds 150 m at the northern end of Yucca Mountain, while at the southern end, the PTn thins to less than 30 m. Within the potential repository area, the thickness of the PTn unit ranges from approximately 60 to 60 m.

From a flow-modeling standpoint, it makes no difference whether a lithostratigraphic representation of the PTn as well as the UZ system is layer-based or spatially distributed in general. Actual models used for such a representation depend primarily on availability of field-specific data. According to the analyses of numerous rock-matrix samples performed by *Flint* [1998], a reasonable one-to-one correlation exists between lithostratigraphic-unit boundaries and hydrogeologic-unit boundaries. In some cases, however, certain lithostratigraphic units within the PTn can be grouped based on similarities in hydrologic properties, while others can be further subdivided. Table 2.1 shows the grouping of layers Tpbt2, Tptrv3, and Tptrv2 into the detailed hydrogeologic unit BT2 (corresponding to UZ model layer ptn26). The hydrologic properties of these layers are not distinct enough to maintain separate hydrogeologic layers [*Flint*, 1998]. The Tpy, on the other hand, shows distinct internal variation in degree of welding beneath the northern portion of Yucca Mountain. Portions of this unit that have porosity values less than or equal to 30% (i.e., the more welded intervals) are identified by a separate hydrogeologic unit [TPY; *Flint*, 1998]. Portions of the Tpy having porosity values greater than 30% are grouped with Tpbt4 or Tpbt3 and identified by hydrogeologic units BT4 and BT3, respectively. As discussed in *Hinds and Pan* [2000], the physical distribution of TPY can only be roughly approximated based on available data. In that report, the TPY is defined as the middle third of lithostratigraphic layer Tpy, but should be considered absent when the thickness of layer Tpy is less than 6 m.

FIGURE 2.2 Geological profile along east-west cross section A-A' (Figure 2.1), taken at a Northing coordinate of 235,119 meters.

FIGURE 2.3 Geological profile along cross section B-B' (Figure 2.1) through borehole UZ-14, taken at a Northing coordinate of 235,087 meters.

FIGURE 2.4 Geological profile along north-south cross section N-S (Figure 2.1), taken at an Easting coordinate of 170,600 meters.

FIGURE 2.5 Geological profile along east-west cross section C-C' (Figure 2.1), taken at a Northing coordinate of 232,000 meters.

As a whole, the PTn unit exhibits very different hydrogeologic properties than the TCw and TSw units that bound it above and below. Both the TCw and the TSw display the low porosity and intense fracturing typical of the densely welded tuffs at Yucca Mountain. Under the current climate and infiltration scenarios, the majority of groundwater flow through these units occurs through fractures. With its high porosity and low fracture intensity, the PTn stands in marked contrast to the welded tuffs. The matrix of the PTn has a large capacity for storing groundwater and is believed to effectively dampen percolation flux at the base of the TCw [Montazer and Wilson]. Moisture imbibing into the PTn matrix from rapid fracture flow of the TCw may result in a more uniform distribution of flux at the base of the PTn.

The potential for capillary-barrier development exists at both upper and lower PTn contacts [Montazer and Wilson, 1984; Flint, 1998]. Rock property contrasts between layers within the PTn unit also have the potential for producing capillary barriers. For flow through single-porosity soils, the extent to which capillary barriers can reduce downward flux and promote lateral diversion depends on saturated hydraulic conductivities of the formation, ambient percolation fluxes, air-entry pressure of the underlying medium, and slopes of the interface between the contrasting layers [Ross, 1990]. Significant lateral flow resulting from capillarity occurs when a fine-textured medium overlies a coarse-textured medium, flux rates are low, and the contact between the two media is linear with a steep slope. Capillary barriers begin to fail (and lateral diversion thus diminishes) when the saturation in the overlying medium increases to a point where the capillary forces are too weak to prevent water from entering the underlying medium (i.e., capillary strength is less than the underlying air-entry pressure).

A complete understanding of groundwater flow behavior within the PTn has proven to be difficult because of extreme heterogeneity in rock properties, resulting from depositional history and post-depositional alteration. Despite the fact that layers within the PTn are laterally continuous and can be relatively easily correlated across Yucca Mountain, their internal hydrologic characteristics may be highly variable. For instance, the Yucca Mountain Tuff (Tpy), which thins dramatically from north to south across the mountain, shows increased welding and devitrification in its interior as the layer thickens. As a result, within this single geologic unit are large variations in porosity, permeability, and fracture characteristics. Currently, the available data on the detailed distribution of rock properties for this unit across the mountain are limited.

Within many of the PTn layers localized zones or intervals of intense smectitic or zeolitic alteration are present. These products have an enormous effect on flow properties and moisture retention characteristics, including permeability, saturation, and capillarity. Vertical and lateral variability in the distribution of mineral alteration occurs on a wide range of scales, making characterization of rock property distribution difficult to assess.

An additional complexity to consider in characterizing general flow behavior (and the capillary-barrier phenomenon in particular) within the PTn unit is the role played by fractures and faults. Given the predominantly nonwelded character of layers within the PTn, fracturing is limited relative to the welded units. Nevertheless, the existence of fractures and faults adds more heterogeneity to the system by interrupting the lateral continuity of rock properties [Day *et al.*, 1998], which reduces the ability of a capillary barrier to laterally diverting water in a large scale. This is an important issue to keep in mind when considering the modeling results presented below.

Hydraulic conductivity within faults is much higher than in surrounding tuffs and is expected to vary along faults, with higher values in the brittle, welded units and lower values in the nonwelded units, where gouge or sealing material may exist [Montazer and Wilson, 1984]. Highly brecciated fault zones may act as vertical capillary barriers to lateral flow, as indicated by high pneumatic permeability measurements in portions of the faults, which suggest large fracture apertures and correspondingly low air-entry pressure. However, if water does enter a fault zone, its high permeability could facilitate rapid vertical flow through the unsaturated system [Wang and Narasimhan, 1988].

The treatment of the effects of major faults on flow is based on the approach used in the UZ flow model [Wu *et al.*, 2000]. This model considers fault zones in the TCw and TSw as intensely fractured conduits for gas flow and for potentially high percolation flux. Fault zones in the PTn are considered less intensely fractured because of the more plastic (non- to partially welded) character of the rock; however, fracturing associated with faulting in the PTn is believed to be still more intense than in unfaulted areas of the PTn. As a result, PTn fracture zones may provide a conduit for gas and liquid flow.

The conceptual model for characterizing the effects of capillary barriers and faults (mainly within the PTn) used in this study is illustrated in Figure 2.6. Three key simplifications made in the development of the conceptual model include: (1) representation of the PTn unit with six internally homogeneous hydrogeologic layers (Table 2.1), (2) representation of layer interfaces as piece-wise linear contacts whose continuity is interrupted only by a few major faults, and (3) representation of faults by vertical columns of gridblocks having finite width (~1 to 10 m). These faults are subdivided vertically into four hydrogeological units, according to their associations with the neighboring major hydrogeological units: TCw, PTn, TSw, and CHn. Under such a conceptualization, capillary barriers may develop at upper, lower PTn contacts, or within the PTn unit, depending on the contrast in hydraulic properties of fractures and matrix as well as moisture conditions between adjacent layers or subunits. Once capillary barriers form along the PTn, significant lateral flow may occur, diverting a large amount of water to faults or to a great distance down the slope.

FIGURE 2.6 Schematic showing the conceptualized flow processes and effects of capillary barriers and major faults within a typical cross section of the UZ flow model domain in the east-west direction.

3. NUMERICAL MODELING APPROACHES

The numerical simulation results presented in this study were carried out using the TOUGH2 and T2R3D codes [Pruess, 1991; Wu *et al.*, 1996]. The flow simulations were performed using an unsaturated flow module of the TOUGH2 code, which solves Richards' equation. Transport runs were carried out by the T2R3D code. The numerical scheme of the TOUGH2 family of codes is based on the integral finite-difference method to solve conservation equations of water and chemical mass components. Such equations are discretized in space using the integral finite-difference method without any reference to a global system of coordinates. This discretization offers the advantage of applicability to regular and irregular geometries of gridding in one, two, and three dimensions. The method also makes it possible, by means of simple preprocessing of geometric data, to implement double- and multiple-porosity or dual-permeability methods for treatment of flow in fractured porous media. In the TOUGH2 formulation, time is discretized fully implicitly, using a first-order backward finite-difference scheme. The resulting discretized finite-difference equations for mass and energy balances are nonlinear and are solved simultaneously using the Newton/Raphson iterative scheme.

Fracture-matrix interactions are handled using the dual-permeability approach (a dual-continuum method) for representing both unfaulted and faulted zones. Both matrix-matrix flow and fracture-fracture flow are considered important to moisture movement in the PTn unit and elsewhere in the unsaturated system of Yucca Mountain. Hence the dual-permeability approach has become the main approach used in the modeling studies for the Yucca Mountain project [Wu *et al.*, 1999]: the dual-permeability methodology considers global flow and transport occurring not only between fractures but also between matrix block connections. In this approach, the formation domain is represented by two overlapping (yet interacting) fracture and matrix continua. Because each fracture gridblock is associated with only one matrix gridblock, fracture-matrix flow must be approximated as quasi-steady [Warren and Root, 1963]. When applied to this study, the traditional dual-permeability concept is further modified using an active-fracture model [Liu *et al.*, 1998] to represent fingering flow effects through fractures. Fracture-matrix flow and interactions with fault domains are also treated using the dual-permeability approach.

3.1 NUMERICAL GRIDS

In the site-scale UZ hydrogeologic model, the PTn unit is represented by six model layers (Table 2.1). The modeling results described in this paper suggest that refined gridding is needed within the PTn to capture detailed flow behavior associated with capillary barriers. To investigate the sensitivity of model results to grid discretization, we generated a small-scale grid 100 m in length and two larger grids 1,000 m in length along cross section A-A' (Figure 2.1). For the 100 m grid, both vertical (Δz) and horizontal (Δx) grid spacings were designed as 1 m (i.e., $\Delta x = \Delta z = 1$ m). Two grids were generated on the 1,000 m scale: one (refined) with a vertical spacing of 1 m ($\Delta z = 1$ m) and a horizontal spacing of 4 m ($\Delta x = 4$ m), the other (coarse) with a vertical spacing of 10 m ($\Delta z = 10$ m) and horizontal spacing of 100 m ($\Delta x = 100$ m). Figure 3.1 shows the refined and coarse grids for the 1,000 m scale model along A-A'. The bottom boundary of each cross section coincides with the interface between the PTn and TSw units. All of the 2-D grids presented in this paper were developed based on rock layer orientations defined in the GFM 3.1 of Yucca

Mountain. Faults were incorporated as vertical zones which penetrate the complete PTn/unsaturated-zone thickness.

Two grids were also made, as shown in Figure 3.2, for the east-west cross section B-B', which passes through borehole UZ-14 (Figures 2.1 and 2.3). The refined grid has $\Delta z = 2$ m and $\Delta x = 10$ m while the coarse grid has $\Delta z = 10$ m and $\Delta x = 100$ m. In each case, the bottom boundary is set at the water table to minimize the boundary effects on flow within the PTn.

Similarly, for the N-S cross section (Figures 2.1 and 2.4), one refined grid is designed with $\Delta z = 2$ m and $\Delta x = 10$ m and one coarse grid is defined with $\Delta z = 10$ m and $\Delta x = 100$ m, as shown in Figure 3.3. For these cross sections, the bottom model boundary is set at the interface between the PTn and TSw units.

Only one grid was developed for the east-west cross section C-C' (Figures 2.1 and 2.5). As shown in Figure 3.4, this grid has $\Delta z = 1$ m and $\Delta x = 10$ m. The bottom model boundary is set at the interface between the PTn and TSw units.

Figure 3.1
UZ2k163

FIGURE 3.1 2-D vertical numerical grids for the 1,000 m scale cross section A-A', (a) refined grid and (b) coarse grid.

Figure 3.2
UZ2k164

FIGURE 3.2 2-D vertical numerical grids for the east-west B-B' cross section through UZ-14, (a) refined grid and (b) coarse grid.

FIGURE 3.3 2-D vertical numerical grids for the north-south (N-S) cross section, (a) refined grid and (b) coarse grid.

FIGURE 3.4 2-D vertical numerical grids for the east-west C-C' cross section through the southern part of the potential repository area.

The numerical grids, as shown in Figures 3.1, 3.2, 3.3 and 3.4, as well as the fracture-matrix characteristic data in Table 3.1 are used to generate dual-permeability meshes. For the dual-permeability treatment, the fractures are considered as a set of uniformly distributed vertical fractures within each of the subunits. Both fracture and matrix gridblocks are globally connected, not only to other fracture and matrix gridblocks within the same unit, but also to those across the boundary of the subunits in the boundary blocks.

TABLE 3.1 Characteristic Data of Fractures with Subunits of TCw and PTn Units.

Subunit	Fracture porosity	Fracture frequency (m^{-1})	Fracture-matrix Interface area (m^2/m^3)
tcw11	2.8E-2	9.2E-1	1.6E+0
tcw12	2.0E-2	1.9E+0	1.3E+1
tcw13	1.5E-2	2.8E+0	3.8E+0
ptn21	1.1E-2	6.7E-1	1.0E+0
ptn22	1.2E-2	4.6E-1	1.4E+0
ptn23	2.5E-3	5.7E-1	1.8E+0
ptn24	1.2E-2	4.6E-1	3.4E-1
ptn25	6.2E-3	5.2E-1	1.1E+0
ptn26	3.6E-3	9.7E-1	3.6E+0

3.2 MODEL BOUNDARY CONDITIONS

For the 2-D grids, model boundaries include the top, bottom, lateral left, and lateral right boundaries. The top model boundary for all the 2-D vertical cross-sectional models coincides with the bedrock surface of the mountain. Surface net-water infiltration is applied to the top boundary using a source term for flow and transport simulations. The bottom boundaries are located either at the bottom of the PTn unit (at the interface between PTn and TSw units) or at the water table. Two types of boundary treatments are adopted for the bottom boundary conditions: one is a Dirichlet-type boundary with constant water pressure (head) specified, the other is a drainage-type boundary along which vertical capillary gradients are set to zero to allow for gravitational drainage flow. For the A-A', C-C', and N-S cross-sectional models, a drainage-type boundary is assigned, while the B-B' model uses a Dirichlet-type boundary.

As shown in Figures 2.2, 2.3, 2.4 and 2.5, the layered tuffs within the unsaturated zone are generally tilted from west to east or from north to south. The lateral or side boundaries of the vertical cross sections may have large effects on lateral flow. In the 2-D models, the up-slope and down-slope boundaries are treated as no-flow (laterally closed) boundaries. This treatment should provide a reasonable approximation to the east-end lateral boundary of the B-B' and C-C' cross sections, because these locations correspond to the "Toe" fault or the Bow Ridge fault. In general, however, the closed boundary treatment will introduce boundary effects and will be discussed in the following sections.

Net infiltration of surface water resulting from precipitation that penetrates the top-soil layer of the mountain is one of the most sensitive factors affecting hydrological behavior within the UZ. Both uniform (5 mm/year) and distributed (based on the estimated surface net-infiltration map) steady-state infiltration rates are used in this work for approximating the present-day mean infiltration [Hevesi and Flint, 2000]. In addition, sensitivity analyses are performed for different values of net infiltration and transient effects.

Before presenting details of modeling studies in the following sections, we must evaluate boundary effects of the 2-D models on modeling results of lateral flow. For bottom boundaries located at the PTn-TSw interface, three types of boundary conditions have been tested, which are: (1) constant head conditions specified using field-measured matrix water potentials, (2) constant head conditions specified using fracture potentials from the UZ flow model [Wu *et al.*, 2000], (3) drainage-type boundary conditions. The modeling results show little difference between the three types of bottom boundary specifications. Furthermore, a model with a bottom boundary extended to the water table gave very similar results to those with bottom boundaries at the PTn-TSw interface. Therefore, the type of bottom boundary condition assigned to the 2-D models has no significant impact on the model results.

The lateral boundary conditions assigned to the right-hand side (or down-slope side) of the east-west cross sections were found to have a significant impact on model results, as observed in a comparison between closed and constant-head types of boundary conditions. Accounting for these effects, the following numerical simulations use drainage-type boundary conditions for bottom boundaries at the PTn-TSw interface and use closed-type conditions for both up-slope and down-slope lateral boundaries.

3.3 FRACTURE AND MATRIX ROCK PROPERTIES

The input parameters for rock and fluid properties include: (1) fracture characteristics (frequency, permeability, *van Genuchten* [1980] α and m parameters, aperture, porosity, and interface area) for each model layer; (2) matrix characteristics (porosity, permeability, and the *van Genuchten* α and m parameters) for each model layer; (3) transport properties (grain density, tortuosity, diffusion, decay and adsorption coefficients) for each model layer; and (4) fault properties (matrix and fracture parameters) for each major hydrogeologic unit. The development and estimation of these parameters for the TCw and PTn units are presented in several related studies [*Ahlers and Liu*, 2000; *Liu et al.*, 2000]. These calibrated rock and fluid properties are used in the present study. Table 3.2 presents the fracture and matrix permeabilities and *van Genuchten's* parameters used for the TCw and PTn units. It is important to note, however, that these calibrated parameters for rock and fluid properties used in this modeling study were developed for the site-scale UZ model [*Ahlers and Liu*, 2000; *Liu et al.*, 2000; *Bandurraga and Bodvarsson*, 1999], which in general had a larger spatial scale than the grid scales in this work.

TABLE 3.2 Modeling Parameter for the TCw and PTn Units

Model Layer/ Hydrogeologic Unit	Matrix Permeability (m ²)	Matrix α (1/Pa)	Matrix m (-)	Fracture Permeability (m ²)	Fracture α (1/Pa)	Fracture m (-)
tcw11	3.86E-15	4.00E-5	0.470	2.41E-12	3.15E-3	0.627
tcw12	2.74E-19	1.81E-5	0.241	1.00E-10	2.13E-3	0.613
tcw13	9.23E-17	3.44E-6	0.398	5.42E-12	1.26E-3	0.607
ptn21	9.90E-13	1.01E-5	0.176	1.86E-12	1.68E-3	0.580
ptn22	2.65E-12	1.60E-4	0.326	2.00E-11	7.68E-4	0.580
ptn23	1.23E-13	5.58E-6	0.397	2.60E-13	9.23E-4	0.610
ptn24	7.86E-14	1.53E-4	0.225	4.67E-13	3.37E-3	0.623
ptn25	7.00E-14	5.27E-5	0.323	7.03E-13	6.33E-4	0.644
ptn26	2.21E-13	2.49E-4	0.285	4.44E-13	2.79E-4	0.552

To investigate the impact of major faults on flow within the PTn, fault properties are also needed. In the conceptual model, as discussed above, faults are represented using a vertical column of finite width (1 m to several m). Fracture-matrix flow and interactions with fault elements are also treated using the dual-permeability approach. Fault properties, estimated using a two-dimensional inversion of saturation, water potential, and pneumatic data [*Ahlers and Liu*, 2000], which was based on the field air permeability test results [*LeCain et al.*, 2000], are listed in Table

TABLE 3.3 Fault Parameters used in the Modeling Studies

Unit	Matrix Permeability (m ²)	Matrix α (1/Pa)	Matrix m (-)	Fracture Permeability (m ²)	Fracture α (1/Pa)	Fracture m (-)
TCw	4.97E-19	9.92E-6	0.181	8.88E-11	3.80E-3	0.633
PTn	1.21E-13	3.71E-5	0.254	2.37E-11	2.80E-3	0.633
TSw	1.11E-15	6.36E-6	0.401	6.38E-11	1.27E-3	0.633
CHn	4.0E-18	9.79E-7	0.386	3.6E-13	2.3E-3	0.633

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4. NUMERICAL RESULTS AND ANALYSES

The modeling studies discussed in this section are conducted for insight into capillary barriers and associated flow behavior within the PTn. These studies are based on the results from a series of 2-D steady-state and transient simulations using different cross sections and infiltration scenarios. As a means of checking numerical results, analytical solutions are developed and use to address the appropriateness of the numerical models for representing the flow system (See Appendix A).

4.1 RESULTS USING 100 M AND 1,000 M SCALE MODELS ALONG A-A'

The simulations discussed in this section are conducted on small-scale models with 100 m and 1,000 m lateral dimensions. The location of the cross sections (A-A', shown in Figure 2.1) is in the northern part of the UZ model domain. Figure 4.1-1(a) and (b) show steady-state percolation fluxes along the PTn-TSw interface, simulated on the two different scales. The figures indicate a significant lateral flow within the PTn models, with a large amount of the percolation flux diverted to a very narrow zone near the down-slope, right-hand boundaries. Lateral flow modeled within the PTn is so strong that infiltration patterns on the ground surface have little impact on flow within the PTn. Percolation flux at the PTn-TSw interface is very similar for the three top-boundary conditions (uniformly distributed infiltration rate of 5 mm/year; focused infiltration on the left-hand side of the model, labeled "left corner injection"; and focused infiltration on the right-hand side of the model, labeled "right corner injection").

Down-slope or right-hand model boundary conditions have a significant impact on model results. For example, the right (down-slope) boundary of the 100 m model would be internal to the 1,000 m model; where the 100 m model predicts large vertical flow (due to ponding), the 1,000 m model predicts small vertical flow. High percolation fluxes simulated near the right-hand side boundary were found to disappear when describing a constant-head condition along the boundary (using steady-state, 1-D flow results). Another phenomenon indicated by Figure 4.1-1 is that lateral flow may also occur in the up-sloping direction because of strong horizontal capillary gradients that overcome gravitational forces, as discussed in *Warrick et al.* [1997]. For the simulation results with point injection (focused infiltration) at the right-hand corner ("Right corner injection"), significant lateral up-slope movement has developed while percolation penetrates the PTn. This large amount of up-slope lateral flow results partially from the description of the vertical, left-hand boundary as a closed boundary, such that a drier or stronger capillary suction region is expected at the up-slope boundary. Physically, the closed vertical boundary may be a good representation of faults at Yucca Mountain.

FIGURE 4.1-1 Simulated vertical percolation fluxes at the PTn-TSw interface along (a) 100 m and (b) 1,000 m scale A-A' cross sections.

Forming a capillary barrier in unsaturated flow through fractured media is more complicated than that in layered or heterogeneous single-continuum porous media or soils [Oldenburg and Pruess, 1993; Ho and Webb, 1998]. Even though capillary barriers in fractured rocks depend also on contrasting hydraulic properties between two contacted layers (as is the case in unfractured soils), capillary barriers in fractured rocks are determined by a combination of vertical capillary gradients in both fracture and matrix systems (as well as interflow between the two continua). Under steady-state flow conditions, local capillary gradients between fractures and matrix tend to be at minimum or near equilibrium, and thus have an insignificant effect on global fracture-fracture or matrix-matrix flow. Therefore, lateral flow is primarily controlled by competing downward gravitational forces and upward capillary gradients in both fractures and matrix systems.

Figure 4.1-2 presents magnitude or norm distributions of the 2-D, steady-state mass flux vector for the 1,000 m scale, A-A' cross section. The modeling results show the importance of two layers: the uppermost PTn layer, ptn21 (corresponding to hydrogeologic unit CNW), and layer ptn23 (corresponding to hydrogeologic unit TPY) (see Table 2.1 and Figure 2.2). Figures 4.1-3 and 4.1-4 show distributions of fracture and matrix capillary pressures, respectively, along the same cross section, indicating significant variations of capillary forces across these two layers, in particular for the matrix capillary pressures (Figure 4.1-3).

A plot of vertical capillary gradients at an Easting coordinate of 171,140 m (Figure 4.1-5) taken from the A-A' cross-sectional model shows the strong capillary-barrier effect in layers ptn21 and ptn23. In the figure, negative capillary pressure gradients are defined for upward flow and positive for downward flow. The upward matrix capillary gradients within layers ptn21 and ptn23 are about 0.1 (bar/m), which is equivalent to the gravity gradient ($\rho_w \times g \approx 0.1$ bar/m). Matrix flow can therefore occur only in the horizontal direction within these layers. Fracture capillary barriers develop within layer ptn23, but not within layer ptn21. Figure 4.1-5 shows that near the

bottom of layer ptn21, fracture capillary gradients are downward. Therefore, within layer ptn21 at the location of this vertical slice, the model predicts counter flow to occur with upward flow in the matrix and downward flow in fractures. The net effect is that overall capillary-barrier effects diminish in this layer.

Figure 4.1-6 presents a locally enlarged flow field for the 2-D pore velocity near the location whose vertical capillary gradients are shown in Figure 4.1-5. Figure 4.1-6 shows large lateral flow along two model layers: the highest velocity grid layers are within layer ptn23, and relatively high velocity zones also appear within layer ptn21.

The strong lateral flow results, as indicated by Figures 4.1-1, 4.1-2, and 4.1-6, imply the dominance of matrix flow within ptn23 and ptn21. Table 3.2 specifies that the van Genuchten α describing capillary functions is more than an order of magnitude lower in the matrix of layer ptn23 compared to the matrix value in the underlying ptn24, indicating that ptn23 has much stronger capillary suction. For fractures, the van Genuchten α is again lower in layer ptn23 than in ptn24, thus favoring the formation of a capillary barrier within the fractures.

FIGURE 4.1-2 Magnitude of simulated 2-D vectors of mass fluxes (kg/s/m^2) for the 1,000 m scale cross section A-A', using the refined grid.

FIGURE 4.1-3 Distribution of simulated matrix capillary pressure (bars) for the 1,000 m scale cross section A-A', using the refined grid.

FIGURE 4.1-4 Distribution of simulated fracture capillary pressure (bars) for the 1,000 m scale cross section A-A', using the refined grid.

FIGURE 4.1-5 Vertical capillary pressure gradients (bar/m) at an Easting coordinate of 171,200 m, from the 1,000 m scale cross section A-A', using the refined grid.

FIGURE 4.1-6 Simulated 2-D flow field within the 1,000 m scale cross section A-A', using the refined grid.

Grid Effects

One of the objectives of this study is to investigate how to represent capillary barrier or lateral flow effects using a large-scale numerical model. A critical question is the effect numerical grid discretization has on modeling results. A series of numerical tests have been completed in an effort to answer this question. Figure 4.1-7 shows some of the results for the 1,000 m scale cross section A-A', in which seven different grids are used with lateral to vertical gridblock dimensions of 4×1 (i.e., $\Delta x = 4$ m and $\Delta z = 1$ m), 10×1, 50×1, 50×5, 100×1, 100×5, and 100×10. Comparison of the simulated percolation fluxes in Figure 4.1-7 indicates a significant effect of grid refinement on modeled results. The results indicate that grid resolution in the vertical direction is more important than in the horizontal direction. If greater than 5 m vertical grid spacing (e.g., $\Delta z = 10$ m) is used, discretization errors are so large that modeled results significantly underestimate lateral flow. This is because several of the PTn layers are thin and would therefore be represented by only one grid layer using $\Delta z \geq 5$ m with the coarse grid (Figure 3.1). Furthermore, certain mobility-weighting or averaging schemes have to be used for evaluating flow coefficients between two adjacent grid layers in a numerical model. It is preferable to discretize at least two numerical grid layers for a single hydrogeologic unit to overcome weighting-scheme effects and to capture capillary-barrier effects. On the other hand, the model results indicate that horizontal gridding can be much more relaxed. Models using Δx values as high as 50 to 100 m still give reasonable answers when compared with results using refined horizontal grid spacings.

FIGURE 4.1-7 Comparison of simulated vertical percolation fluxes at the PTn-TSw interface along the 1,000 m scale A-A' cross section using different grid discretizations.

Grid effects on modeled results of lateral flow can also be seen from the magnitude distribution of simulated mass flow, as displayed in Figure 4.1-8. Compared with Figure 4.1-2 the figure indicates much smaller lateral flow with a coarse grid, within layer ptn23. The simulated

vertical gradients of capillary pressures from the coarse grid are much weaker than those shown with the refined grid (Figure 4.1-5) because certain key layers, such as ptn23, are represented by only one grid layer in the coarse-grid model.

FIGURE 4.1-8 Distribution of simulated 2-D vectors of mass fluxes (kg/s/m^2) for the 1,000 m scale cross section A-A', using a coarse ($\Delta x = 100 \text{ m}$, $\Delta z = 10 \text{ m}$) grid.

Sensitivity to Fracture Properties

The influence of PTn fracture properties on lateral flow effects is considered an important issue in site characterization studies of Yucca Mountain because field data regarding fracture moisture flow are limited. The two-phase fracture flow properties are largely determined through inverse modeling using matrix moisture and pneumatic data [Ahlers and Liu, 2000]. Therefore, significant uncertainties may exist associated with estimated values of fracture properties in the PTn unit. Two sensitivity analyses are performed here: one uses arithmetically averaged absolute fracture permeability and the van Genuchten a parameter for the six hydrogeologic units, comprising the PTn. The other takes out fractures completely from the PTn because of the nonwelded nature of the unit and the fact that few fractures are observed to be present in the unit.

Figure 4.1-9 presents simulated percolation fluxes along A-A' at the PTn-TSw interface from the two sensitivity analyses, and compares these results with the results of model simulations using on the fracture data in Table 2.1. Note that even with significant modifications in fracture properties for the two cases, all three models predict very similar flux patterns or lateral flow effects from the PTn unit. This suggests the uncertainties in fracture properties of the PTn unit may not be very critical to modeling results in terms of moisture flow through the PTn unit.

FIGURE 4.1-9 Comparison of simulated vertical percolation fluxes at the PTn-TSw interface along the 1,000 m scale A-A' cross section using different fracture properties.

Transient Infiltration

The net surface infiltration at the bedrock surface (top of the TCw unit) is conceptualized as episodic, with significant pulses probably occurring once every few years [Hevesi and Flint, 2000]. Spatially and temporally variable pulses of moisture percolate rapidly through the highly fractured tuffs of the TCw, as indicated by the numerous bomb-pulse chlorine-36 signatures measured within the TCw [Fabryka-Martin, 2000]. However, at the TCw-PTn interface, where welded tuffs grade sharply into nonwelded tuffs, flow behavior changes from fracture-dominated to matrix-dominated flow [Wu *et al.*, 2000]. The highly porous PTn unit may also attenuate the episodic infiltration flux significantly, such that the net episodic surface infiltration, once crossing the Ptn, may be approximated as steady state.

Effects of surface transient infiltration on capillary barriers and percolation are here analyzed using numerical models. We use a 50 m long, 2-D section model (or half) of the 100 m (A-A') cross section and a 1-D model at the Easting coordinate of 170,906 m. Surface infiltration pulses are assumed to be uniformly distributed spatially with a one-week infiltration cycle during 50 years, i.e., the model top boundary is subject to nonzero infiltration for only one week every 50 years. The net infiltration value of the week, averaged over the 50 years, is also at 5 mm/yr. The initial conditions for both the 2-D and 1-D models correspond to steady-state under 5 mm/yr infiltration.

Figure 4.1-10 presents simulated bottom percolation fluxes at different times, as compared with the initial steady-state results. Figure 4.1-10 indicates that simulated percolation fluxes at the PTn-TSw interface vary with times under transient pulses of infiltration, but the magnitude of the transient variation of the fluxes at the bottom of the PTn is relatively small compared with the

pulses on the surface. The strong effect of capillary barriers on transient percolating fluxes is evident because very similar flow patterns resulted for all the times. Figure 4.1-11 shows the variations of total fluxes at the bottom of the PTn, as well as surface infiltration pulses, versus time from the 2-D and 1-D models. A comparison of surface infiltration patterns and bottom fluxes (Figure 4.1-11) clearly implies the importance of damping effects of the PTn unit. Surface transient infiltration pulses can be significantly smoothened temporally after the early transient period of several hundreds of years. Note that Figure 4.1-11 presents the results for up to 1,000 years, following the steady-state flow, initial condition. After rapid changes during the first several hundreds of years, the total fluxes at the bottom boundaries gradually approach the average value of 5 mm/yr, and eventually the system should reach a dynamic equilibrium condition under the uniform pulses of infiltration.

FIGURE 4.1-10 Simulated vertical percolation fluxes at different times across the PTn-TSw interface along a 50 m long section of the 100 m scaled A-A' cross section.

FIGURE 4.1-11 Simulated variations in total percolation fluxes versus times at the bottom PTn unit of the 2-D and 1-D models.

4.2 RESULTS USING CROSS-SECTIONAL MODELS ALONG B-B'

The difference between east-west cross section B-B' and cross section A-A' is the larger spatial scale of B-B', which crosses the entire UZ model domain and contains three vertical faults, as shown in Figures 2.1 and 2.3. Vertically, this cross-sectional model covers the entire UZ with the bottom boundary located at the water table. Two numerically discretized grids (Figure 3.2) are used to represent the B-B' cross section. The refined grid has $\Delta x = 10$ m and $\Delta z = 2$ m, while the coarse grid has $\Delta x = 100$ m and $\Delta z = 10$ m. Two types of net surface infiltration are used for the top model boundary condition: a uniformly distributed (5 mm/year) rate and a spatially variable rate extracted from the U.S. Geological Survey present-day infiltration map [Hevesi and Flint, 2000].

Cross section B-B' is considered more representative for use in modeling large-scale flow behavior because it includes several major faults and has a larger spatial scale in both vertical and horizontal directions than cross section A-A'. In an effort to examine the model results of moisture flow, we compare modeled predicted saturations of matrix liquid to the observation data, as shown in Figure 4.2-1. This figure indicates that although the simulated matrix liquid saturations are in reasonable agreement with measured values for both types of surface infiltration (i.e., uniform and distributed), the results using the distributed infiltration provide a better match. At the bottom of the PTn unit, however, modeled saturations are higher than the field data. This may be a limitation of the 2-D model because results using a 3-D model [Wu *et al.*, 2000] have been able to better match the data.

FIGURE 4.2-1 Comparison of simulated and observed matrix liquid saturations for borehole UZ-14, using the refined grid with uniform and distributed surface net infiltration (averaging 5 mm/yr).

The simulated percolation flux at the PTn-TSw interface along B-B' is shown in Figures 4.2-2 and 4.2-3, using the two grids and two types of surface net infiltration scenarios. The figures reveal significant lateral flow diversion occurring within the PTn, with a large amount of water being diverted to down-slope faults (e.g., Solitario Canyon, Ghost Dance and Drill Hole Wash faults). Therefore, faults become major flow pathways crossing the PTn under the current conceptual model. Again, the coarse grid significantly underestimates lateral flow or capillary-barrier effects. Comparison of the simulated flux patterns at the PTn-TSw interface in Figures 4.2-2 and 4.2-3 shows that they are very similar for the two infiltration cases. This indicates that knowledge of detailed spatial distributions of net surface infiltration may not be critical, once percolating waters have traveled to the base of the PTn unit. From a performance standpoint, Figures 4.2-2 and 4.2-3 show that the simulated percolation flux directly above the potential repository (in the area between the Solitario Canyon and Ghost Dance faults) is significantly reduced by lateral diversion to faults for both infiltration scenarios. Simulated percolation flux also becomes more smoothly or uniformly distributed after crossing the PTn unit in unfaulted zones (for the distributed surface infiltration scenario using the refined grid model results).

FIGURE 4.2-2 Simulated vertical percolation flux at the PTn-TSw interface along B-B' using refined and coarse grids with uniform surface net infiltration (averaging 5 mm/yr).

FIGURE 4.2-3 Simulated vertical percolation flux at the PTn-TSw interface along B-B' using refined and coarse grids with distributed surface net infiltration (averaging 5 mm/yr).

The effects of capillary barriers and faults on flow along B-B' can be clearly seen from distributions in magnitude of the 2-D, steady-state mass flux vector in Figure 4.2-4. The figure again identifies layers ptn23 and ptn21 as controlling the lateral flow within the PTn unit. The figure also shows that major faults provide the main flow pathways for vertical percolation flux. Only one high vertical flux zone, at an Easting coordinate of 172,000 m (between Ghost Dance and Drill Hole Wash faults) is not related to faults. In this area, layers ptn21 and ptn23 become very thin (~ 2 m, see Figure 2.3). A weaker capillary-barrier effect is therefore expected. In this case, even the refined grid may be too coarse in this area.

FIGURE 4.2-4 Magnitude of simulated 2-D vectors of mass flux (kg/s/m^2) along B-B' using the refined grid and uniform surface infiltration.

Effects of Net Infiltration

The simulation results discussed above indicate that net infiltration values have more overall impact on capillary barriers or lateral flow than detailed spatial distributions of infiltration along the model top boundary. Figure 4.2-5 compares the impact of net infiltration rates on percentage of flow through faults and fault zones. In the figure, faults include the Solitario Canyon, Drill Hole Wash, Pagany Wash and "Toe" (eastern boundary) faults, and fault zones are defined as fault columns plus a 20 m wide zone west (up-slope) of each fault. As net infiltration increases, the percentage of fault flow decreases. This happens because both fractures and rock matrix in areas between faults become wetter with increased net infiltration, leading to generally weaker capillary barriers between rock layers and consequently less lateral diversion of moisture to fault zones.

Figure 4.2-5 also shows that about 25% of the percolation flux has been laterally diverted into faults within the PTn. Including the 20 m faults zones, fault flow consists of about 40% of the total flow at lower infiltration rates. Note that this result comes from averaging over the entire

cross section; therefore, fault flow percentage for the domain directly above the repository is much higher (Figures 4.2-2 and 4.2-3).

FIGURE 4.2-5 Effects of net infiltration values on percentage of flow through faults and fault zones, reflecting amount of lateral water flow within the PTn unit along the B-B' cross, using the refined grid and uniform surface infiltration pattern.

Transport

These analyses are based on transport simulations of a conservative tracer to obtain insight into groundwater travel times and radionuclide transport from the bedrock surface to the bottom of the PTn unit. The same refined and coarse, east-west (B-B') cross-sectional grids (with the dual-permeability modeling approach) are used in the transport calculations.

The tracer is treated as a conservative (nonadsorbing) component transported through the model. The hydrodynamic dispersion effect through the fracture-matrix system is found to be insensitive to modeled results [Wu *et al.*, 2000] and is ignored. A constant molecular diffusion coefficient of $3.2 \times 10^{-11} \text{ m}^2/\text{s}$ is used for matrix diffusion, and K_d (sorption coefficient) is set to zero. Two transport simulations were run to 100,000 years under steady-state flow fields and initial, constant source concentration conditions in the fracture blocks at the top model boundary. This implies that a tracer is instantaneously released at the starting time of a simulation.

Tracer transport or groundwater travel times can be analyzed using a cumulative or fractional breakthrough curve, as shown in Figure 4.2-6. The fractional mass breakthrough in the figure is defined as the cumulative mass of tracer arriving at the PTn-TSw interface over time, normalized by the total initial mass introduced at the surface. The figure shows that it takes two to three thousands of years for groundwater to travel across the PTn if we use 50% mass breakthrough for averaging travel times. Figure 4.2-6 also shows that the coarse grid predicts a longer travel time of

3,400 years versus 2,700 years estimated with the refined grid, because the coarse grid predicts less lateral diversion to faults, or less fast flow. The tracer transport time at 50% breakthrough may be used as an indicator to water ages in the formation. Carbon composition (^{14}C) data, collected within the bedded tuffs of the PTn unit near this cross section (B-B') from 1984 to 1994 [Yang *et al.*, 1996], gives average activity values of 70 pmc (percent modern carbon). This corresponds to about 2,900 years of water ages and therefore indicates that the tracer-transporting modeling results are consistent with the field data.

Figure 4.2-7 presents the spatial distribution of cumulative mass per unit area along the PTn-TSw interface, normalized to its highest value, at 100% mass breakthrough. This figure shows tracer breakthrough locations along the cross section and again identifies the faults as major transport pathways through the PTn. Comparison of mass breakthrough areas in Figure 4.2-7 with flux distributions in Figures 4.2-2 and 4.2-3 shows a very similar pattern. This indicates that the transport process is dominated by advection.

FIGURE 4.2-6 Simulated fractional breakthrough curves of cumulative tracer mass arriving at the PTn-TSw interface (since releasing from the surface), along the B-B' cross section, using the refined and coarse grids and uniform surface infiltration pattern.

FIGURE 4.2-7 Simulated distributions of cumulative tracer mass arriving at the PTn-TSw interface along the B-B' cross section, using the refined and coarse grids and uniform surface infiltration pattern.

4.3 RESULTS USING CROSS-SECTIONAL MODELS ALONG N-S

As shown in Figures 2.1, 2.4 and 3.3, the N-S cross section vertically transects the repository area from north to south and has its bottom boundary at the base of the PTn unit. This cross section contains only one fault (the Drill Hole Wash fault) in the north of the model domain. Both uniform and distributed infiltration maps are specified along the top model boundary. Two numerical grids (Figure 3.3) are developed for the cross section: a refined grid with $\Delta x = 10$ m and $\Delta z = 2$ m, and a coarse grid with $\Delta x = 100$ m and $\Delta z = 10$ m.

The simulated percolation flux at the PTn-TSw interface using refined and coarse grids along the N-S cross section is shown in Figures 4.3-1 and 4.3-2, respectively. The figures show that significant lateral flow diversion occurs only in the northern part of the model domain, about one third of the total cross-sectional length. This is because layers ptn21 and ptn23 are thicker and more steeply dipping to the south (Figure 2.4). The Drill Hole Wash fault behaves as a major flow pathway in this northern area. In the southern portion of the model cross section (Northing coordinate $< 234,000$ m), little lateral flow is observed in the figures because layers ptn23 and ptn21 become very thin or pinch out, and the units lie flatter (Figure 2.4).

Figure 4.3-3 presents a magnitude distribution of the simulated mass flux vector within the N-S model, showing again that the ptn23 and ptn21 layers contribute the most to lateral flow along this section (mainly in the northern half of the model). Grid resolution effects can be analyzed by comparing flow patterns in Figures 4.3-1 (refined grid) and 4.3-2 (coarse grid). In the northern part, the coarse-grid model underestimates lateral flow or capillary-barrier effects, while in the

south the refined-grid model results in a much smoother flux variation along the PTn-TSw interface than the coarse model. This indicates that percolation fluxes are effectively damped spatially when simulated using the refined-grid model. In contrast, the coarse-grid model (Figure 4.3-3) shows a flux pattern at the PTn-TSw interface similar to the surface infiltration in the southern half of the model under both uniform and distributed surface infiltration conditions. Therefore, no effective percolation damping is obtained using the coarse grid.

FIGURE 4.3-1 Simulated vertical percolation flux at the PTn-TSw interface along the N-S cross section using uniform and distributed surface infiltration (both averaging 5 mm/yr) and the refined grid.

FIGURE 4.3-2 Simulated vertical percolation flux at the PTn-TSw interface along the N-S cross section using uniform and distributed net surface infiltration (both averaging 5 mm/yr) and the coarse grid.

FIGURE 4.3-3 Magnitude of simulated 2-D vectors of mass flux (kg/s/m^2) within the N-S cross section, using the refined grid and uniform surface infiltration.

4.4 RESULTS USING CROSS-SECTIONAL MODELS ALONG C-C'

The vertical cross section C-C' (Figures 2.1 and 2.5) is used to investigate potential lateral flow occurring in the east-west direction in the southern part of the potential repository area (at a Northing coordinate of 232,000 m). As shown in Figure 2.5, rock layers dip to the east and are intersected by two major faults (Ghost Dance and Imbricate faults).

As with the other cross-sectional models, the top boundary of the C-C' model is described using uniform and distributed net infiltration over the model domain. Both scenarios have average net infiltration rates of 5 mm/yr. The bottom model boundary coincides with the PTn-TSw interface and is described by a drainage condition. The numerical grid (Figure 3.4) for cross section C-C' is discretized with $\Delta x = 10$ m and $\Delta z = 1$ m.

Figure 4.4-1 displays the simulated percolation flux at the PTn-TSw interface along C-C' for the two infiltration scenarios. The figure shows considerable lateral flow, particularly in the eastern half of the model. In the area directly above the potential repository (i.e., to the west of the Ghost Dance fault), the extent and amount of lateral flow, however, is smaller than in the northern B-B' cross section (see Figures 4.2-2 and 4.2-3). This is because the PTn unit is very thin beneath southern Yucca Mountain (~30 m, Figures 2.4 and 2.5), and layer ptn23 has pinched out. Figure 4.4-2 indicates that capillary effects are mainly contributed by layer ptn21, which is uniform along the entire cross section. In the eastern part of the cross section, the layers dip more steeply to the east, and more lateral flow is expected. Again, the Ghost Dance and Imbricate faults serve as major flow pathways along this section.

FIGURE 4.4-1 Simulated vertical percolation flux at the PTn-TSw interface along the C-C' cross section using uniform and distributed surface infiltration (both averaging 5 mm/yr).

FIGURE 4.4-2 Magnitude of simulated 2-D vectors of mass flux (kg/s/m^2) within the C-C' cross section using the uniform surface infiltration.

5. ANALYTICAL ANALYSES

In addition to the numerical modeling studies discussed above, analytical solutions are obtained (Appendix A) under steady-state flow in fractured media using the ECM assumption. These analytical solutions and a simplified flow system are used to further analyze capillary-barrier effects at Yucca Mountain. The simplified flow system consists of only two layers and is assumed to be infinite laterally and vertically. The interface between the two layers dips at a constant angle of 5.55° . Fracture and matrix properties for ptn23 and ptn24 (see Tables 3.1 and 3.2) are assigned to the two layers.

Figure 5.1 presents profiles of capillary heads under different infiltration scenarios, calculated using analytical solutions. As shown in Figure 5.1, ambient infiltration rates have significant impact on capillary head distributions in the upper layer for the two-layer system with the given properties. Figure 5.2 shows vertical capillary pressure-head gradients under the same infiltration rates as in Figure 5.1, indicating influence of capillary-barrier zone thickness (defined as a zone with capillary head gradient values in a range of -1 to 0). As discussed in Section 4.1, when the gradient is -1, capillary barriers reach a physical maximum that will completely overcome gravity effects. In this case, flow occurs only in the horizontal direction. If the gradient is zero, then capillary-barrier effects no longer exist. In general, as infiltration rates increase, as shown in Figure 5.2, capillary-barrier zones get smaller.

Effects of capillary barriers may be quantified using Figure 5.3. In the figure, the ratio (m^2) of total lateral flow (integrated over a 20 m thickness above the interface) to surface infiltration rates is a measure for intensity or strength of capillary-barrier effects under consideration. Physically, this ratio of lateral flow to infiltration rate correlates total lateral flow over a certain depth to net surface infiltration values, and it roughly reflects how large surface areas, with a given infiltration rate, must be to satisfy the total lateral flow by the capillary barrier. Therefore, the larger the ratio of lateral flow to infiltration rate, the larger the capillary-barrier or lateral-flow effects. For a 2-D flow system such as the one being studied, the ratio is equivalent to a lateral flow length, or how long the upstream slope should be to receive enough infiltrated water for the amount of lateral flow to occur. Figure 5.3 shows that there is almost a linear relationship between infiltration rates and the ratio. For example, a lateral flow length of about 1,000 m is needed for a 10 mm/yr infiltration rate. This indicates significant capillary-barrier effects exist for the system if infiltration rates are 10 mm/yr or smaller.

Note that the analytical approach is based on many simplified assumptions, and that the resulting analyses may not be representative to describing flow within the PTn unit at Yucca Mountain. However, in a general sense, the fundamentals and insights from the analytical solutions should be useful to further numerical modeling or field investigations.

FIGURE 5.1 Profiles of capillary pressure heads in the upper layer of the two-layer system under different infiltration rates, calculated using analytical solutions.

FIGURE 5.2 Profiles of vertical capillary pressure gradients in the upper layer of the two-layer system under different infiltration rates, calculated using analytical solutions.

FIGURE 5.3 Ratio of total lateral flow integrated over 20 m thickness above interface to infiltration rates, measuring intensity of capillary or lateral flow effects, calculated using analytical solutions.

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6. DISCUSSION

The unsaturated hydrogeologic system beneath Yucca Mountain, and specifically within the PTn unit, is highly heterogeneous on any model scale. Order-of-magnitude contrasts in permeability exist between rock layers as well as between fracture and matrix systems within the rock. Layer dip and continuity are variable, reflecting geologic deposition and subsequent deformation caused by uplift and faulting. Consequently, the capillary-barrier phenomenon in the UZ at Yucca Mountain is particularly complex compared to those capillary barriers in unsaturated porous soils.

Two-phase flow functions of relative permeability and capillary pressure determined for Yucca Mountain tuffs are extremely nonlinear and highly contrasting between fracture and matrix continua. As a result, flow through fractures and matrix blocks are on very different time scales (e.g., fracture flow may be hundreds of times faster than matrix flow). On the other hand, fractures have a much smaller storage space and much weaker capillary suction than the matrix. Global moisture flow through fractured rocks is contributed by both fracture-fracture and matrix-matrix flow, which is also affected by fracture-matrix interflow. Furthermore, characterizing the flow patterns through the PTn is complicated by the existence of numerous faults, which cross the entire PTn unit, interrupt possible lateral flow, and provide downward flow pathways for infiltrating water.

Modeling results using site-specific data confirm that significant lateral flow develops in the presence of layered rock with contrasting hydraulic properties, low percolation flux, and sloping, linear layer interfaces. Effective capillary barriers are primarily determined by a combination of both matrix and fracture capillary gradients. If two capillary gradients point to the same, upward direction, strong capillary barriers may form. Under certain circumstances, two capillary gradients can cancel each other and counter flow may occur through the two continua, which makes net capillary effects weak.

This study indicates that under the current hydrogeologic conceptualization of the unsaturated zone at Yucca Mountain, strong capillary-barrier effects exist within layers ptn21 and ptn23 for diverting moisture flow through the PTn unit. A map showing the approximate extent of layer ptn23 [TPY; Clayton, 2000] within the UZ flow model domain is shown in Figure 6.1, indicating that this layer is only present in the northern repository area. The numerical studies presented above show that capillary barriers or lateral flow in the PTn unit is controlled mainly by the ptn23 layer in the north and by the ptn21 layer in the south. Water may be diverted hundreds to thousands of meters laterally along these two layers unless intercepted by major faults. Faults serve as major downward pathways for laterally diverted water, and faults themselves may behave as capillary barriers to down-slope lateral flow from up-slope regions.

FIGURE 6.1 Approximate extent of layer ptn23 (corresponding to hydrogeologic unit TPY) within the PTn unit of the UZ flow model domain.

The sensitivity analyses conducted in this work indicate that it takes several thousands of years for 50% of the groundwater to travel through the PTn. Capillary barriers within the PTn unit are mainly controlled by contrasts in matrix hydraulic parameters, while fracture properties have a less significant impact on moisture flow. Average net infiltration rates, not detailed spatial distributions, have a larger impact on flow patterns through the PTn unit. Both numerical and analytical models show that capillary-barrier effects are strongly correlated with surface infiltration rates, with lower infiltration leading to larger lateral flow. As net infiltration rates increase, the system gets wetter and capillary barriers become weaker as a result. Numerical grid resolution is important for capturing the effects of thin layers on the formation of strong capillary barriers. For large-scale modeling, limitations on vertical grid spacing are more important than on horizontal spacing. No more than 5 m vertical grid spacing should be used for the upper portion of the PTn unit. In addition, strong capillary-barrier effects exist within the PTn under transient, pulsed infiltration, and the PTn is very effective in damping transient infiltration pulses spatially and temporally in the unfaulted zones.

7. CONCLUSIONS

A systematic modeling study of capillary barriers is presented for unsaturated flow in fractured rocks, using the site-specific data from Yucca Mountain. The modeling results indicate that with the current conceptualization, significant capillary-barrier effects exist and large-scale lateral flow within the PTn unit occurs as a result. This work demonstrates that a capillary barrier in unsaturated fractured rocks is determined by a combination of matrix-matrix and fracture-fracture flow fields and, therefore, is a more complicated phenomenon than in single porous media.

The modeling investigation of capillary barriers and lateral flow constitutes an important step in characterizing fluid flow processes within Yucca Mountain. This study provides certain insights into the flow behavior and the roles of the PTn unit. However, considerable uncertainties still remain in our understanding of the unsaturated hydrogeologic system at Yucca Mountain. In terms of relative importance, this study identifies two critical areas affecting lateral diversion of moisture flow: (1) two key subunits, ptn23 and ptn21, of the PTn unit and (2) faults, which may limit the extent of lateral flow and which may themselves play a role in the formation of capillary barriers. Future work should be focused on characterizing the two layers as well as faults for their detailed spatial variations and flow properties. Furthermore, field studies, such as collecting geochemical data in the areas near faults and far away from faults, may provide more information regarding water ages, important for estimating groundwater travel times or establishing occurrences of lateral flow.

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APPENDIX A: DERIVATION AND EVALUATION OF ANALYTICAL SOLUTIONS

Assuming a local thermodynamic or capillary equilibrium condition between fracture and matrix continua, the effective continuum method (ECM) can be used to describe unsaturated flow in fractured rocks. Under such a flow condition, the Richards' equation can be written in the same form (pseudo one-dimensional flow) in terms of the ECM formulation [Wu, 1999] and for flow in a single-continuum porous medium [Philip, 1991]:

$$\frac{\partial(\phi S_w)}{\partial t} = \frac{\partial}{\partial n} \left[K(h) \frac{\partial h}{\partial n} \right] + \frac{\partial K(h)}{\partial n} \cos(\beta) \quad (\text{Eq. 1})$$

where, ϕ , S_w , h , t , n , and β are effective porosity, water saturation, capillary pressure head, as well as time, the normal coordinate, and the angle of the layer interface, respectively. $K(h)$ is effective hydraulic conductivity, as a function of capillary pressure. Note that n is measured upwards and perpendicular to the interface.

Equations (A-1) contains several "effective" or "equivalent" parameters and constitutive correlations that need to be determined [Wu, 1999]. The effective porosity is defined as,

$$\phi = \phi_f + \phi_m \quad (\text{Eq. 2})$$

where ϕ_f and ϕ_m are effective porosities of fracture and matrix continua, respectively. The effective water saturation is

$$S_w = \frac{S_{w,f} \phi_f + S_{w,m} \phi_m}{\phi_f + \phi_m} \quad (\text{Eq. 3})$$

where $S_{w,f}$ and $S_{w,m}$ are water saturation in fracture and matrix continua, respectively. The effective hydraulic conductivity is

$$K(h) = K_{f,s} k_{rf}(h) + K_{m,s} k_{rm}(h) \quad (\text{Eq. 4})$$

where $K_{f,s}$ and $K_{m,s}$ are saturated hydraulic conductivities and k_{rf} and k_{rm} are the relative permeability to water for fracture and matrix continua. Note that under the capillary equilibrium assumption, pressure heads in fractures and matrix are the same locally, and Equations (2), (3) and (4) provide a complete set of constitutive correlations for solving Equation (1).

In the ECM formulation, the problem, as described by Equation (1), for flow through unsaturated fractured rocks, becomes equivalent to that through porous soils [Warrick *et al.*, 1997]. Therefore, the analytical solutions derived by Warrick *et al.* [1997] may be directly extended to the case of

fractured media using the ECM approximation. The pressure profile for an infinite slope/interface is then described by

$$h = h_1 \quad n \leq 0 \quad (\text{Eq. 5})$$

and

$$n \cos(\beta) = \int_{h_1}^h \frac{dh}{\frac{q}{K_2(h) - 1}} \quad n > 0 \quad (\text{Eq. 6})$$

where the subscripts 1 and 2 denote the lower and upper layers, respectively, q is the infiltration rate and $K_2(h)$ is the effective hydraulic conductivity of the upper layer. The total horizontal flow Q_h can be calculated as

$$Q_h = -\tan(\beta) \int_{h_1}^{h_2} K_2(h) dh \quad (\text{Eq. 7})$$

Note that these results do not assume any particular form of hydraulic conductivity $K(h)$ relationships.

The analytical solutions of (5), (6), and (7), are extended directly from those for flow in single-continuum porous media and are only valid under the ECM assumption. We must check the analytical solutions for their applicability to fractured media with or without assuming local capillary equilibrium. Here we use numerical solutions to examine the above analytical solutions. A large 2-D model domain 4,400 m long and 382 m high is used to approximate an infinite two-dipping layer system, with the upper layer 380 m thick. The domain is discretized using a rectangular grid with grid spacings between 1 to 100 m along the sloping direction and between 0.1 to 10 m in the direction perpendicular to the sloping. The parameters used for the two layers are those for ptn23 and ptn24, as given in Tables 3.1 and 3.2. The dipping angle of the interface or the slope is 5.55° , and the infiltration rate is uniformly 5 mm/yr. In numerical solutions, both dual-permeability and ECM conceptual models are used for handling fracture-matrix flow.

Comparisons between the results from analytical and numerical solutions are shown in Figure A-1. For numerical solutions using the dual-permeability approach (2k), only matrix pressure heads are plotted. Figure A-1 indicates that the analytical solutions are in excellent agreement with numerical simulations, using both dual-permeability and ECM formulations. This examination shows that the analytical solutions are applicable to the fractured-flow situation with or without the capillary equilibrium assumption for the PTn system under study. The comparison also indicates that the ECM provides a good approximation to modeling steady-state flow. Furthermore, Figure A-1 indicates that the numerical grid resolutions and results of this work are proper for the problems under study because similar model grids and parameters were used for all the numerical studies.

FIGURE A.1 Comparison of pressure head profiles in the PTn2 layer, calculated using the analytical and numerical solutions.