Modeling capillary barriers in unsaturated fractured rock

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[1] This work presents a series of numerical modeling studies that investigate the hydrogeologic conditions required to form capillary barriers and the effect that capillary barriers have on fluid flow and tracer transport processes in the unsaturated fractured rock of Yucca Mountain, Nevada, a potential site for storing high-level radioactive waste. The modeling approach is based on a dual-continuum formulation of coupled multiphase fluid and tracer transport through fractured porous rock. The numerical modeling results showed that effective capillary barriers can develop where both matrix and fracture capillary gradients tend to move water upward. Under the current hydrogeologic conceptualization of Yucca Mountain, strong capillary barrier effects exist for diverting a significant amount of moisture flow through the relatively shallow Paintbrush nonwelded unit, with major faults observed at the site serving as major downward pathways for laterally diverted percolation fluxes. In addition, we used observed field liquid saturation and goechemical isotopic data to check model results and found consistent INDEX TERMS: 1829 Hydrology: Groundwater hydrology; 1832 Hydrology: Groundwater agreement. transport; 1866 Hydrology: Soil moisture; 1875 Hydrology: Unsaturated zone; KEYWORDS: capillary barriers, unsaturated zone, fractured porous media, Richards' equation, dual-continuum model

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1. Introduction

[2] It has been recognized that capillary barriers may form under unsaturated conditions in layered, porous soils and formations [e.g., *Miyazaki*, 1988; *Ross*, 1990]. Studies of the formation of capillary barriers under unsaturated conditions in layered, fractured rock [*Montazer and Wilson*, 1984] closely relate to the unsaturated zone (UZ) flow and transport site-characterization efforts for the fractured tuffs at Yucca Mountain, Nevada. Located in the arid western United States, the thick UZ 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.

[3] The natural capillary barrier concept has been of considerable interest during the performance assessment phase for the potential repository. Capillary barriers can 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] hypothesized that capillary barriers exist at layer contacts where a unit with relatively small (fine) pores or fractures. More recent studies include an estimation of lateral diversion capacity, using an analytical approach [*Wilson*, 1996], and numerical modeling, using a layered, porous medium model [*Moyer et al.*, 1996].

[4] Quantitative analysis of capillary barriers (and resultant lateral flow) has previously been performed using

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analytical approaches [Ross, 1990; Morel-Seytoux et al., 1996; Warrick et al., 1997; Webb, 1997; 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 of these investigations have focused primarily on the generation of capillary barriers resulting from the contrasting 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.

[5] Despite the progress made in the understanding of capillary barriers in porous soils over the last several decades, very few studies have focused on the capillary barrier phenomenon in fractured rock. During early site characterization of the UZ at Yucca Mountain, the capillary barrier concept was proposed and assessed conceptually [Montazer and Wilson, 1984]. Subsequent numerical modeling investigations [Rulon et al., 1986; Wittwer et al., 1995; Moyer et al., 1996; Wu et al., 1999, 2002] have shown a wide range of variability in the amount of lateral flow associated with capillary barrier or permeability-barrier effects in unsaturated fractured tuffs. Consequently, a general need has arisen for an in-depth analysis of the fundamental controlling factors related to the generation of capillary barriers in fractured media.

[6] Many types of field data have been collected from the Yucca Mountain site over the past two decades. These data have been used to formulate a conceptual model and understanding of the mountain's hydrologic system. A



Figure 1. Plan view of the UZ model domain, showing the model boundary, the potential repository outline, major fault locations, selected boreholes, and the location of vertical cross sections used in this paper.

comprehensive, three-dimensional, UZ flow model based upon the previously characterized hydrologic units has been developed for the unsaturated system [*Wu et al.*, 2000, 2002]. This model allows for the exploration of various flow phenomena such as capillary barrier formation (and resultant lateral diversion into existing faults) and tracer transport times to key layer boundaries under different spatial distributions of surface infiltration.

[7] The systematic modeling study presented in this paper investigates the capillary barrier phenomenon in fractured rock using three two-dimensional (2-D), vertical cross-sectional models that incorporate site-specific data from Yucca Mountain. The modeling approach is based on a dual-permeability conceptual model for handling fracture and matrix flow and interaction [*Wu et al.*, 1999]. The objectives of this work are to investigate: (1) what needs to be accounted for when using the dual-permeability model to simulate the development of capillary barriers, (2) where capillary barriers of varying effectiveness may develop at

Yucca Mountain, based on the current hydrogeologic conceptual model, (3) which controlling factors are responsible for the formation of capillary barriers at the site, and (4) what effect the capillary barriers have on the system as a whole. In addition, we will also check model results against observed field data of liquid saturation and goechemical isotopic data.

2. Hydrogeologic Setting and Conceptual Model

[8] As shown in Figure 1, the aerial domain of the UZ model encompasses approximately 40 km² of the Yucca Mountain area [*Hinds and Pan*, 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. Subsurface hydrologic processes in the UZ occur in a heterogeneous environment of layered, anisotropic, fractured volcanic rock [*Scott and Bonk*, 1984], consisting of alternating layers of welded and nonwelded ash-flow and

Table 1. Major Hydrogeologic Units, Geologic Units, UZ ModelLayers, and Detailed Hydrogeologic Unit Correlation Used in thePTn Flow Studies

Major Hydrogeologic Unit	Geologic Unit	UZ Model Layer
Tiva Canyon welded (TCw) Tiva Canyon welded (TCw) Tiva Canyon welded (TCw) Paintbrush nonwelded (PTn) Paintbrush nonwelded (PTn) Paintbrush nonwelded (PTn) Paintbrush nonwelded (PTn) Paintbrush nonwelded (PTn) Paintbrush nonwelded (PTn)	Tiva Canyon Tuff Tiva Canyon Tuff Tiva Canyon Tuff Diva Canyon Tuff bedded tuff Yucca Mountain Tuff bedded tuff Pah Canyon Tuff Bedded tuff Topopah Spring Tuff	tcw11 tcw12 tcw13 ptn21 ptn22 ptn23 ptn24 ptn25 ptn26 ptn26

air-fall tuffs. The major units have been reorganized into major hydrogeologic units based roughly on the degree of welding within each unit [*Montazer and Wilson*, 1984]. These units are (1) the Tiva Canyon welded (TCw) unit; (2) the Paintbrush nonwelded (PTn) unit, which consists primarily of the Yucca Mountain and Pah Canyon tuffs and their bedded tuffs; (3) the Topopah Spring welded (TSw) unit; (4) the Calico Hills nonwelded (CHn) unit; and (5) the Crater Flat undifferentiated (CFu) unit.

[9] The subdivision of hydrogeologic units in this study follows the scheme of the current UZ flow model [*Hinds* and Pan, 2000; Wu et al., 2000], which is in turn based on the current geologic framework model (GFM) of Yucca Mountain by Clayton [2000] and the analysis of rock property data by Flint [1998]. In the geologic model, the UZ system 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. Table 1 correlates geologic units with hydrogeologic units and shows the UZ model grid layer names for the section of the UZ at Yucca Mountain above the TSw unit.

[10] Figure 1 also displays the locations of three east-west cross sections through the northern part of the potential repository area along three transects (A-A', B-B', and C-C'). Transect A-A' has a lateral scale of 1000 (1000 m scale) and lies between the Solitario Canyon and Drill Hole Wash faults. Transect B-B' has a lateral scale on the order of 4000 m (UZ model scale) and crosses a series of major faults (Figure 1), while Transect C-C' has a 3000 m scale along the dipping slope of the PTn unit in the northwest–southeast direction.

[11] Figure 2 illustrated a typical geologic profile along vertical east-west transects (e.g., B-B') as well as the conceptual model that characterizes the potential effects of capillary barriers and faults on the UZ system. The PTn unit, focus of this study, consists primarily of nonwelded to partially welded tuffs. The dip of these layers is generally less than 10° to the east or southeast. The combined thickness of the PTn layers is from 150 m in north to 30 m in south. The PTn unit as a whole exhibits very different hydrogeologic properties from 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. In contrast, the PTn has high porosity and low fracture intensity; and its matrix system has a large capacity for storing groundwater; it has been shown to effectively dampen percolation flux at the base of the TCw [Montazer and Wilson, 1984].

[12] In previous studies [*Montazer and Wilson*, 1984; *Flint*, 1998], capillary barriers were speculated to exist at both upper and lower PTn contacts, because of the large contrast in rock properties across the interfaces of the unit. In addition, rock property contrasts between sublayers within the PTn unit may potentially produce capillary



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Figure 2. Schematic showing the conceptualized flow processes and effects of capillary barriers and major faults within a typical east-west cross section of the UZ model domain.

barriers. Characterization of groundwater flow behavior within the PTn is critically dependent on knowledge of rock properties and the heterogeneity within the PTn unit. The field data, obtained from tens of boreholes and hundreds of outcrop samples at the site, help constrain the distribution of rock properties within the PTn unit. In general, field data indicate that the formation is more heterogeneous vertically than horizontally, with layer-wise representations providing reasonable approximation of the complex geologic system. This is because many calibration results using this conceptual model could match different types of observation data [Wu et al., 2000]. However, characterizing general flow behavior (and the capillary barrier phenomenon in particular) within the PTn unit may be complicated by the presence of faults, which add more heterogeneity to the system by interrupting the lateral continuity of rock matrix properties [Day et al., 1998].

[13] The key conceptualizations made in the conceptual model of this study are as follows: (1) The hydrogeological units/layers are internally homogeneous and the material properties of each unit (defined by previously calibrated parameters [*Ahlers and Liu*, 2000]) are continuous throughout each layer (Table 1), unless interrupted by faults; (2) Ambient water flow in the system is at a steady state condition; and (3) Faults are represented by vertical columns of gridblocks having finite width.

[14] At Yucca Mountain, permeability within faults is much higher than that in the surrounding fractured tuffs and is expected to vary along faults [*Montazer and Wilson*, 1984]. In addition, pneumatic permeability measurements taken along portions of faults have revealed low air-entry pressures, indicating that large fracture apertures are present in the fault zones [*Ahlers and Liu*, 2000]. Therefore pore size in fault zones is expected to be larger than that outside fault zones, leading to weaker capillary forces, with such fault zones possibly acting as vertical capillary barriers to lateral flow. If water does enter a fault zone, however, its high vertical permeability could facilitate rapid vertical flow through the unsaturated system [*Wang and Narasimhan*, 1988]. Faults are treated as highly fractured zones with different fracture-matrix properties [*Wu et al.*, 2002].

3. Numerical Modeling Approaches

[15] The numerical simulation results presented in this study were carried out using the TOUGH2 simulator, which solves the Richards' equation for flow simulations [*Pruess*, 1991], and the T2R3D code, which solves coupled fluid flow and transport for tracer transport runs [*Wu et al.*, 1996]. Fracture-matrix interactions are handled using the dual-permeability approach (a dual-continuum method) for representing both unfaulted and faulted zones. Because of the known low percolation flux at the site, matrix-matrix flow and fracture-fracture flow are both considered to be important to moisture movement in the UZ system of Yucca Mountain. Hence the dual-permeability approach has become the main method used in modeling studies for the Yucca Mountain site [*Wu et al.*, 1999].

3.1. Numerical Grids

[16] To investigate the sensitivity of model results to resolution of grid discretization, we experimented with using different gridding refinements for discretizing the vertical

Table 2. Spatial Resolution of 2-D Grids Designed for Discretizing the Three Vertical Cross Section Models

	Coarse		Refined		
Cross Section\Grid	Horizontal (Δx) , m	Maximum Vertical (Δz), m	Horizontal (Δx) , m	Maximum Vertical (Δz), m	
A-A' B-B' C-C'	100 100	10 10	4 10 10	1 2 3	

cross-sectional models. Table 2 lists examples of grid spatial resolution used in this study for the three cross sections (A-A', B-B', C-C' of Figure 1). Horizontal grid spacings are designed as uniform, while vertical ones are variable, dependent on the thickness of geological layers in an effort to reserve the stratigraphic information or actual thickness of the geological layers. We have conducted many more numerical experiments on grid refinement versus capturing capillary effects and found that use of sufficient grid discretization is crucial to modeling capillary barrier phenomena.

3.2. Model Boundary Conditions

[17] Model boundaries include the top, bottom, lateral left, and lateral right sides. The top boundary for all of the cross-sectional models coincides with the bedrock surface of the mountain. Two types of surface infiltration are used for the top boundary condition: (1) a uniformly distributed (5 mm/year) rate and (2) a spatially variable rate extracted from the U.S. Geological Survey present-day infiltration map [*Hevesi and Flint*, 2000]. In addition, sensitivity analyses are performed for different values of net uniform infiltration rates.

[18] The bottom boundaries of the A-A' and C-C' cross sections are designed to simulate drainage at the PTn-TSw interface. Along the interface boundary, vertical capillary gradients are set to zero to allow for free gravitational drainage flow (or drainage-type boundary). The B-B' model uses a Dirichlet-type boundary at the water table. We have evaluated the effect of using different bottom boundary conditions at the PTn-TSw interface, specifying (1) constant-head conditions using field-measured matrix water potentials, (2) constant-head conditions with fracture potentials from the UZ flow model [Wu et al., 2000], and (3) drainage-type conditions. The sensitivity results show little difference in simulated values of percolation flux, water potential and saturation 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 for the same model domain.) Thus the type of bottom boundary condition assigned to the 2-D models has no significant impact on the model results; only the grid blocks very close to the bottom boundary are affected.

[19] The layered tuffs within the UZ generally dip to the southeast. The lateral (i.e., side) boundaries of the vertical cross sections may have a large effect on lateral flow. In the 2-D models, no flow is allowed crossing the upslope and downslope side boundaries. This treatment should provide a reasonable approximation of the three selected east bound lateral boundary of the A-A', B-B' and C-C' cross sections, because these locations are at or close to faults. Where the

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

Table 3. Modeling Parameters for the TCw and PTn Units^a

^aRead 3.86E-15 as 3.86×10^{-15} .

boundary is far away from faults, however, these lateral noflow boundaries, without allowing continuous lateral flow across them, will introduce boundary effects. A sensitivity analysis using a vertically varying head condition (obtained from a large-scale model result for the same location), instead of a closed boundary, indicates that in the 2-D model the lateral closed boundary treatment introduces errors only to a small spatial range within 50 meters from the boundary.

3.3. Fracture and Matrix Properties

[20] The input parameters for the rock and fluid properties of the TCw and PTn used in the model were estimated in several related studies [*Ahlers and Liu*, 2000]. Rock properties include fracture frequency and fracture-matrix permeability, van Genuchten [1980] α and m parameters, aperture, porosity, and interface area. Table 3 presents the permeability and van Genuchten parameters for the fracture and matrix components of the TCw and PTn units. To investigate the impact that major faults have on flow and transport within the PTn, we additionally need the fracture and matrix properties of the faults within the system. These fault properties were previously estimated using a 2-D inversion of liquid saturation, water potential, pneumatic, and air-permeability data [*Ahlers and Liu*, 2000].

4. Results and Analyses

[21] The modeling results discussed in this section are based upon the three cross-sectional 2-D steady state models discussed above and mainly focus on the development of capillary barriers and their associated flow and transport behavior within the PTn unit. The first (A-A') cross-sectional model is used to analyze the fundamentals of capillary barrier phenomena in fractured formation. The second (B-B') model is for insight of a larger, mountain scale behavior as well as effects of major faults at the Yucca Mountain site, while the third (C-C') cross section discusses effect of small faults and tracer transport.

4.1. Results Using the 1000 m (Small Scale) Model Along A-A'

[22] Figure 3 presents the 2-D, steady state, mass flux vector magnitude distribution for the 1000 m wide A-A' cross section (Figure 1). Dark zones indicate high flow rates. The modeling results shown in Figure 3 illustrate the importance of two layers: (1) ptn21 (the uppermost PTn layer) and (2) ptn23 (see Table 1). Significant lateral flow

occurs along these two layers within the PTn unit because strong capillary barriers have developed directly below these units. Note that a large amount of the percolation flux is diverted into a very narrow zone near the downslope, right-hand boundaries, which is due to the artificial effect of a no lateral flow boundary there.

[23] The modeling results from the A-A' cross section indicate that the process of forming a capillary barrier in fractured media is more complicated than in layered or heterogeneous single-continuum porous media or soils [Oldenburg and Pruess, 1993; Ho and Webb, 1998]. Capillary barriers in either fractured rock or unfractured soils depend on contrasting hydraulic properties between two contacted layers. However, the formation of capillary barriers in fractured rock is dependent not only on the interaction of vertical capillary gradients in both fracture and matrix systems of the layer, but also on the interflow between the two continua. Under steady state flow conditions, local capillary gradients between the fractures and matrix tend to be at a minimum (relative to transient flow) or near equilibrium. These gradients have little effect on global fracture-fracture or matrix-matrix flow. Thus lateral flow is primarily controlled by the net effect of competing downward gravitational forces and upward capillary gradients in both fracture and matrix systems.

[24] Figure 4 further illustrates the effect that the interactions of the two continua have on the development of capillary barriers. In Figure 4, vertical capillary gradients at an easting coordinate of 171,140 m of the A-A' cross section are plotted for the fracture and matrix continua of the model. In addition, the two layers previously shown (in Figure 3) to exhibit a strong potential capillary barrier effect (ptn21 and ptn23) are indicated. Negative capillary pressure gradients on Figure 4 imply upward vertical flow, and positive capillary pressure gradients indicate downward vertical flow, as would be driven by capillary gradients alone. Both capillary gradients and gravitational forces drive actual flow. The upward vertical matrix flow within layers ptn21 and ptn23 exhibits capillary pressure gradients of approximately ~ 0.1 (bar/m). These upward gradients are balanced by the gravity gradient ($\rho_w \times g \approx 0.1$ bar/m), such that matrix flow can occur only in the horizontal direction within these two layers. In a similar manner, capillary barrier effects in the fracture continuum are expected at the base of layer ptn23, where upward vertical fracture flow (i.e., a negative capillary pressure gradient) is again balanced by the downward gravitational gradients. Layer



Figure 3. 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.

ptn21, on the other hand, exhibits an unbalanced downward flow by capillary gradients in the fracture continuum, and thus the capillary barrier effect in this layer is diminished (Figure 3). Strong fracture-matrix counter flow is also seen at a lower elevation of 1240 m, which explains why no lateral flow occurs at that level (Figure 3). [25] The 2-D flow field shown in Figure 5 confirms that large lateral flow is indeed occurring along the ptn21 and ptn23 model layers, reaching maximum flow velocities within ptn23. Table 3 specifies that both the fracture and matrix van Genuchten α (5.58 × 10⁻⁶ and 9.23 × 10⁻⁴) (which describes capillary functions) for layer ptn23 are



Figure 4. Vertical capillary pressure gradients (bar/m) at an Easting coordinate of 171,200 m from the 1000 m scale cross section A-A', using the refined grid.

35 - 7



Figure 5. Simulated 2-D flow field within the 1000 m scale cross section A-A', using the refined grid.

much lower than that for the underlying ptn24 values (1.53 $\times 10^{-4}$ and 3.37 $\times 10^{-3}$). This indicates that ptn23 is expected to have a very strong capillary suction, as indicated by the large capillary pressure contrast shown along the ptn23-ptn24 boundary in Figure 5.

[26] The influence of fracture properties on capillary barrier effects is further investigated by several sensitivity analyses using the A-A' cross-sectional model. We used arithmetically averaged absolute fracture permeability and the van Genuchten m parameter of relative permeability for the six hydrogeologic units comprising the PTn. We found that even with significant modifications in fracture properties, model results predict very similar flux patterns or lateral flow effects in the PTn unit to the results discussed above. The most critical parameter of fractures to impact the formation of a capillary barrier is the van Genuchten α for the fracture-matrix system under study. In addition, we experimented with using a different modeling approach to handle fracture-matrix interaction the double-porosity method (i.e., ignoring the global matrix-matrix connection, while retaining the same fracture-matrix properties). The model results show a larger sensitivity to modeling approaches than to fracture properties. Without global matrix flow, very small lateral flow or capillary barrier effect is predicted with the double-porosity model. This is because, in this case, all global flow occurs through fractures only, and the contrast in fracture properties in the PTn layers is too small to form a strong capillary barrier. This also suggests that the matrix system, with its stronger capillary forces, plays a dominant role in controlling lateral flow through the PTn unit.

[27] Another objective of this study is to investigate how to accurately represent capillary barrier formation (and the

resultant lateral flow effects) using a large-scale numerical model. To better understand the effect that grid discretization has on the model results, we have performed a series of numerical tests in which we use a variety of grid cell sizes for the A-A' cross-sectional model. Seven different grids of varying vertical and horizontal grid-cell sizes (i.e., lateral to vertical grid-cell 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) are explored. Comparison of the simulated percolation fluxes using the different grids indicates that grid refinement has a significant effect on modeled results. In particular, grid resolution in the vertical direction has a more significant impact on model results than in the horizontal direction. Use of the "coarse" model is in general unable to fully capture the amount of lateral flow within the critical PTn unit, because several PTn sublayers are too thin to be properly represented with coarse grids (e.g., using $\Delta z \ge 5$ m). On the other hand, model results indicate that horizontal grid-cell spacing is not as critical. Models using Δx values as high as 50 to 100 m with the 2-D models still give results similar to those using more refined horizontal grid cells.

4.2. Results Using Cross-Sectional Model Along B-B'

[28] Cross section B-B' (Figure 1) is considered more representative than cross section A-A' in modeling largescale flow behavior, because it includes several major faults and covers the entire thickness of the UZ. Figure 6 compares observed values of matrix liquid saturation measured in borehole UZ-14 (Figure 1) with simulated results to assess how well the models are estimating moisture flow. Above the base of the PTn ($z = \sim 1,260$ m), the simulated matrix liquid saturations are in reasonable agreement with



Figure 6. 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 observed values regardless of the type of surface infiltration used (although the distributed infiltration model provides a slightly better match). At the bottom of the PTn unit, however, modeled saturation values are substantially higher than the field data. This limitation may be because a 2-D model is used. The 3-D model of *Wu et al.* [2000] has been able to better match the field data at these elevations.

[29] Comparison of percolation flux values at the top and the bottom of the PTn allows for an estimation of the

amount of lateral flow occurring within the unit. Model results show that percolation patterns along the top of the PTn are essentially the same as surface infiltration. Consequently, the following analyses simply use surface infiltration values as proxy for the actual percolation occurring at the top of the PTn. Figure 7 compares these distributed surface infiltration values with the modeled percolation flux at the PTn-TSw interface (bottom of the PTn) along B-B' for both the coarse and refined grids. Figure 7 shows that significant lateral flow diversion is occurring within the PTn and that a large amount of the water is being diverted downslope to the Solitario Canyon, Ghost Dance, and Drill Hole Wash faults. The large difference in model results (of simulated percolation fluxes and their distribution along the PTn-TSw interface using the refined and coarse grids) indicates the importance of grid refinement. The coarse grid may not adequately estimate the amount of lateral flow in the system. Figure 7 also shows 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 the lateral diversion of water into faults. In addition, the percolation values become more uniform in the unfaulted zones after passing through the PTn. Seepage into the repository is less likely to occur when water flux in the region above is more uniform near the mean value [Finsterle, 2000]. It should also be noted that when a uniform surface infiltration is used, both the coarse and fine model results along the PTn-TSw boundary are similar to those shown in Figure 7. Therefore knowledge of detailed spatial distributions of surface net infiltration may not be critical once percolating waters have traveled to the base of the PTn unit.

[30] The effects of capillary barriers and faults on flux values along B-B' are evident in Figure 8, which plots the magnitude of the 2-D steady state mass flux vectors for the entire cross section. As expected, layers ptn23 and ptn21 are controlling the lateral flow within the PTn unit. Figure 8



Figure 7. 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).



Figure 8. Magnitude of simulated 2-D vectors of mass flux (kg/s/m²) along B-B' using the refined grid and uniform surface infiltration.

further confirms that major faults are providing the main flow pathways for vertical percolation flux (see also Figure 7). 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 fault infiltration. In this area, layers ptn21 and ptn23 become very thin (~2 m) and a weaker capillary barrier effect in this region is therefore expected.

[31] Although the spatial distribution of surface infiltration has little or no impact on the distribution of flow at the base of the PTn, simulation results indicate that net infiltration values have more of an overall impact on capillary barriers (and lateral flow). As net infiltration increases, the percentage of fault flow decreases, because both fractures and matrix in the unfaulted areas become more saturated with increase in net infiltration. The more saturated the system is, the generally weaker the capillary barriers between rock layers become. Consequently, there is less lateral diversion of moisture into fault zones. For this particular section, the model results show that an average of $\sim 20\%$ of the total percolation flux has been laterally diverted into faults or fault zones in high-infiltration scenarios, and fault flow consists of $\sim 40\%$ of the total flow at lower-infiltration rates.

4.3. Results Using Cross-Sectional Model Along C-C'

[32] This cross-sectional model is used to examine effects of small faults and to investigate tracer transport or groundwater travel times under strong lateral flow conditions. As shown in Figure 1, this cross section is oriented from northwest to southeast, which in general follows the dipping direction of the PTn unit in this area. The geologic model indicates that it intersects several small faults (defined as vertical faults with small, ~ 1 m offsets, not shown in Figure 1), in addition to one major fault (Drill Hole Wash). Two numerical grids with the same resolution (Table 2) were generated for this cross section, one explicitly including the



Figure 9. Comparison between simulated vertical percolation fluxes at the PTn-TSw interface along C-C' with and without including small faults (averaging 5 mm/yr).



Figure 10. Simulated normalized tracer concentration breakthrough curves at three elevations of x = 1300 m, along the middle of the C-C' cross section.

one major fault and seven small faults and the other only the major fault. In the model, both major and small faults were treated as vertical zones with 2 m width. The difference is in assignment of fracture-matrix properties to fault zones, in which the major fault uses calibrated fault fracture-matrix properties, while small faults incorporate only calibrated fault fracture properties, with their matrix having the same properties as those of the adjacent unfaulted matrix blocks.

[33] Figure 9 shows a comparison of percolation flux values and patterns simulated along the PTn-TSw interface or bottom boundary, with and without small faults. The two simulations use the same uniform surface infiltration of 5 mm/yr, specified along the top boundary. Figure 9 also indicates the locations of eight faults (one major and seven small faults). Note that Figure 9 shows a similar flux pattern along the PTn-TSw interface with and without incorporating small faults, except in the areas near faults. The smallfault model results show higher fluxes on upslope sides and lower fluxes on downslope sides near or at small faults, owning to lateral capillary barrier effects in those small

faults. On the other hand, the non-small-fault model predicts much higher percolation fluxes at the major fault and the eastern boundary (also a fault), since they are the only vertical fault zones within the cross section to provide fast flow pathways.

[34] A further examination of the two model results indicates that small faults, where they exist, interrupt continuous lateral flow. However, existence of small faults affects only the small regions in the immediate vicinity (<50 m) of these faults. The model may still provide good estimates of average fluxes, even though it fails to include these small faults when no sufficient fault characterization data are available. In both cases, significant lateral flow occurs in the unfaulted regions along this cross section of the PTn unit. Also, when checking fluxes by mass balance in the eastern portion beyond the major fault, we observe that water partially flows across small and major faults laterally. In other words, within this cross section faults are not completely diverting lateral flow.

[35] In the (C-C') cross-sectional model, transport simulations of a tracer are presented for further insight into capillary barrier effect on groundwater travel times and radionuclide transport in the PTn unit. The tracer is treated as a conservative (nonabsorbing) component transported through the model. The mechanical dispersion effect through the fracture-matrix system was previously found to be insensitive to modeled results [Wu et al., 2002] and is ignored in this study. (A constant molecular diffusion coefficient of 3.2×10^{-11} m²/s is used for matrix diffusion.) Two transport simulation scenarios of different tracer release were run to 100,000 years under steady state flow fields (generated by the flow model including small faults). The first scenario releases tracer with initial constant-source concentration in fracture blocks along the entire top model boundary, and the second releases tracer with initial constant-source concentration at only one fracture block of the top (x = 200 m).

[36] For the first scenario, the tracer transport or groundwater travel times are analyzed using breakthrough curves of concentrations (Figure 10), monitored at several elevations within the PTn at x = 1,300 m in the middle of the cross section model. Figure 10 shows that it takes 2000– 3000 years for groundwater to travel to these depths, as indicated by peak values of concentration breakthrough curves. Note that in Figure 10 the first peak at ptn25 (z =



Figure 11. Distribution of normalized tracer concentrations within the C-C' cross section percolation after 1000 years of tracer release from the one-point source.

1,210 m) corresponds to travel times of the tracer released from the top-boundary area directly above the observation point, while the second, higher peak is the result of combined downward and laterally diverted transport. Carbon composition (¹⁴C) data, collected within the bedded tuffs of the PTn unit near this cross section (C-C') from 1984 to 1994 [*Yang et al.*, 1996], reveal average activity values of 70 pmc (percent modern carbon). This corresponds to a water age of ~2,900 years in the PTn, similar to that predicted by the model. This result supports the model prediction that significant lateral movement and mixing may occur in the PTn.

[37] Figure 11 displays a snapshot of normalized tracer concentration (relative to initial source concentration C_0) distributions in fractures after 1000 years of tracer release, indicating significant lateral flow or transport along the cross section from the second transport simulation. At the same time, the simulated matrix concentration plume is similar to the one (Figure 11), but a little delayed in travel distance. The results of the second simulation indicate that the center of the tracer plume, upon reaching the PTn-TSw interface, has moved laterally about 1000 m along the cross section, with the plume front laterally crossing several faults. The average groundwater travel times to the bottom boundary, estimated from the second, one point tracer release simulation, is much longer than those from the first simulation with uniform tracer release on the top. This is because the one-point tracer release result predicts a much longer travel distance than the average results of the uniform tracer release scenario under the same flow conditions.

4.4. Discussion

[38] The unsaturated hydrogeologic system beneath Yucca Mountain (specifically within the PTn unit) is spatially highly heterogeneous. Contrasts in permeability are much larger between neighboring rock layers than within the same rock unit. Layer dip and continuity are variable, reflecting geologic deposition and subsequent deformation caused by uplift and faulting. In short, the capillary barrier phenomenon in the unsaturated fractured rocks at Yucca Mountain is very difficult to characterize.

[39] Modeling results using site-specific data demonstrate that significant lateral flow develops in the presence of layered rock that exhibits contrasting fracture-matrix hydraulic properties, low percolation flux, and sloping layer interfaces. Effective capillary barriers occur when upward capillary gradients exist for fractures and the matrix. Counter flow with in the two continuua, if occurs, can weaken the net capillary effects. This study indicates that under the current hydrogeologic conceptualization of the UZ at Yucca Mountain, strong capillary barrier effects exist within layers ptn21 and ptn23 for diverting moisture flow through the PTn unit, especially in the northern repository area. Our numerical studies show that capillary barriers (and resultant lateral flow) in the PTn unit is controlled mainly by the ptn23 layer in the north and (more weakly) by the ptn21 layer in the south from additional model studies. Based on the current uniform layer-wise property conceptualization, the model indicates that water could be diverted hundreds to thousands of meters laterally along these two layers unless intercepted by faults. Major faults serve as major downward pathways for laterally diverted water, and faults themselves

may behave as capillary barriers to downslope lateral flow. On the other hand, sensitivity analysis indicates that small faults, serving as fast flow pathways, have an insignificant impact on percolation patterns at the PTn-TSw interface.

[40] This study also indicates that, on average, it takes several thousand years for groundwater to travel through the PTn. Average net infiltration rates (not detailed spatial distributions) have a larger impact on flow patterns through the PTn unit. Capillary barrier effects are strongly correlated with surface infiltration rates: lower net infiltration leads to relatively larger lateral flow. Fracture properties, except van Genuchten α , are insensitive to forming a strong capillary barrier for the system under study. We also found that the resolution of numerical grids used in modeling studies must be refined enough to capture the formation of strong capillary barriers within thin layers. For large-scale modeling, vertical grid refinement is more important than horizontal spacing.

[41] In addition to agreement between model results and matrix field saturation and water age data (Figures 6 and 10), independent evidence also suggests that lateral flow occurs in the UZ of Yucca Mountain. Measured pore water chemical compositions obtained from boreholes scattered throughout Yucca Mountain are similar for the same lithologic units [Yang et al., 1998], especially in the PTn. The uniformity in chemical composition for each geologic layer supports the model indications of strong lateral interactions within the PTn layer. If lateral flow were not occurring, we would expect that the chemical compositions derived from the pore water data in these layers would be nonuniformly distributed according to surface infiltration pattern. I. C., Yang (Percolation flux and transport velocities in the unsaturated zone, Yucca Mountain, Nevada, submitted to Applied Geochemistry, 2001) uses ¹⁴C residence times of pore water and water content measurement to obtain two estimates of percolation fluxes at UZ-14. Both estimates show that percolation fluxes in the TSw are considerably lower than in the upper, PTn unit, which provides more direct evidence for lateral flow within the PTn.

5. Summary and Concluding Remarks

[42] A systematic modeling study of capillary barriers is presented for unsaturated flow in fractured rock, using the site-specific data from Yucca Mountain. The modeling results indicate that significant capillary barrier effects exist and result in large-scale lateral flow within the PTn unit. This work shows that capillary barrier formation in unsaturated fractured rock is determined mainly by a combination of matrix-matrix and fracture-fracture flow fields and thus is a more complicated phenomenon than that described for porous soils. Model results demonstrate that numerical modeling approaches, in particular tracer transport analyses, provide a powerful and convenient tool to characterize capillary barrier phenomena in fractured rock.

[43] The modeling investigation of capillary barrier formation and resultant lateral flow constitutes an important step in characterizing the fluid flow processes within Yucca Mountain. This study provides insights into UZ flow behavior and the role of the PTn unit for lateral flow. However, considerable uncertainties still remain in our understanding of the unsaturated hydrogeologic system at Yucca Mountain. For future research efforts, this study identifies two critical geologic features affecting lateral diversion of moisture flow at Yucca Mountain: (1) two key subunits of the PTn unit (ptn21 and ptn23) and (2) faults, which may limit the horizontal extent of lateral flow and may themselves play a role in the formation of vertical capillary barriers. Future work should be focused on characterizing the spatial variations and flow properites of the two key PTn layers. To better estimate groundwater travel times and to more fully confirm the occurrence of lateral flow, geochemical water-age data both near and far from faults at Yucca Mountain should be collected in future field studies.

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