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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET

Complete Only Applicable Items

1. QA: QA JEH 4/21/00

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2. ☐ Analysis Check all that apply

Type of Analysis
- ☐ Engineering
- ☐ Performance Assessment
- ☐ Scientific

Intended Use of Analysis
- ☐ Input to Calculation
- ☐ Input to another Analysis or Model
- ☐ Input to Technical Document

Describe use:

3. ☒ Model Check all that apply

Type of Model
- ☒ Conceptual Model
- ☐ Abstraction Model
- ☐ Mathematical Model
- ☐ System Model
- ☐ Process Model

Intended Use of Model
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Describe use:

Provides conceptual models for UZ models documented in other AMRs and in the UZ PMR.

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Conceptual and Numerical Models for UZ Flow and Transport

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD
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1. Page: 2 of: 60

2. Analysis or Model Title:

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CONTENTS (Continued)

FIGURES

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ACRONYMS

ACC	Accession Number
AMR	Analysis/Model Report
AP	Administrative Procedure
CFu	Crater Flat Undifferentiated Hydrogeologic Unit
CHn	Calico Hills nonwelded hydrogeologic unit
CRWMS	Civilian Radioactive Waste Management System
CPU	Central Processing Unit
DOE	Department of Energy
DST	Drift Scale Test
ECM	Effective Continuum Method
ESF	Exploratory Studies Facility
LBNL	Lawrence Berkeley National Laboratory
MINC	Multiple Interacting Continua Approach
M&O	Management and Operating Contractor
OCRWM	Office of Civilian Radioactive Waste Management
PA	Performance Assessment
PMR	Process Model Report
PTn	Paintbrush nonwelded hydrogeologic unit
QAP	Administrative Procedure (M&O)
QARD	Quality Assurance Requirements and Description
QIP	Quality Implementing Procedure
TBV	To Be Verified
TC	Thermal-Chemical
TCw	Tiva Canyon welded hydrogeologic unit
TDMS	Technical Data Management System
THC	Thermal-Hydrologic-Chemical
TH	Thermal-Hydrologic
TM	Thermal-Mechanical
TSw	Topopah Spring welded hydrogeologic unit
UZ	Unsaturated Zone
YMP	Yucca Mountain Site Characterization Project

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1. PURPOSE

The purpose of this Analysis/Model Report (AMR) is to document the conceptual and numerical models used for modeling of unsaturated zone (UZ) fluid (water and air) flow and solute transport processes. This is in accordance with *AMR Development Plan for U0030 Conceptual and Numerical Models for Unsaturated Zone (UZ) Flow and Transport Processes, Rev 00* (CRWMS M&O 1999c). The conceptual and numerical modeling approaches described in this AMR are used for models of UZ flow and transport in fractured, unsaturated rock under ambient and thermal conditions, which are documented in separate AMRs. This AMR supports the UZ Flow and Transport Process Model Report (PMR), the Near Field Environment PMR, and the following models:

- Calibrated Properties Model
- UZ Flow Models and Submodels
- Mountain-Scale Coupled Processes Model
- Thermal-Hydrologic-Chemical (THC) Seepage Model
- Drift Scale Test (DST) THC Model
- Seepage Model for Performance Assessment (PA)
- UZ Radionuclide Transport Models

Conceptual models for flow and transport in unsaturated, fractured media under ambient and thermal conditions are discussed in terms of their applicability to the UZ at Yucca Mountain. The rationale for selecting the conceptual models used for modeling of UZ flow and transport at the drift- and mountain-scale is documented. Numerical approaches for incorporating these conceptual models are evaluated in terms of their representation of the selected conceptual models and computational efficiency. The rationales for selecting the numerical approaches used for modeling of UZ flow and transport are also documented.

Caveats and limitations include use of the van Genuchten relation for the active fracture continuum, use of porous-medium equivalence for describing flow and transport in fracture networks, and the assumption of steady-state liquid flow in the UZ. More discussions on these caveats and limitations are presented in Sections 5 and 6 of this AMR.

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2. QUALITY ASSURANCE

This AMR was developed in accordance with AP-3.10Q, *Analyses and Models*. Other applicable Department of Energy (DOE) Office of Civilian Radioactive Waste Management (OCRWM) Administrative Procedures (APs) and YMP-LBNL Quality Implementing Procedures (QIPs) are identified in *AMR Development Plan for U0030 Conceptual and Numerical Models for Unsaturated Zone (UZ) Flow and Transport Processes, Rev 00* (CRWMS M&O 1999c).

The activities documented in this AMR were evaluated with other related activities in accordance with QAP-2-0, Conduct of Activities, and were determined to be subject to the requirements of the U.S. DOE OCRWM Quality Assurance Requirements and Description (QARD) (DOE 1998). This evaluation is documented in CRWMS M&O (1999a, 1999b) and Wemheuer (1999) (Activity Evaluation for Work Package WP 1401213UM1).

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3. COMPUTER SOFTWARE AND MODEL USAGE

No modeling studies or computer simulations were performed for this AMR, and therefore no software codes, macros, or routines were used. However, this AMR does present the numerical methods that are the basis of the software codes used in the AMRs that support the UZ PMR. Likewise, the conceptual models presented in this AMR are the basis for the models that support the UZ PMR. All of the modeling studies referred to in Section 6 were performed as part of other AMRs, and the status of the software used for the studies is specified in those AMRs.

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4. INPUTS

4.1 DATA AND PARAMETERS

No data from the Technical Data Management System (TDMS) are directly used. This AMR documents the approaches utilized for modeling UZ flow and transport processes and does not provide model output and numerical simulations.

4.2 CRITERIA

This AMR complies with the DOE interim guidance (Dyer 1999). Subparts of the interim guidance that apply to this analysis or modeling activity are those pertaining to the characterization of the Yucca Mountain site (Subpart B, Section 15) and the definition of conceptual models used in performance assessment (Subpart E, Section 114(a)).

4.3 CODES AND STANDARDS

No specific formally established standards have been identified as applying to this activity.

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5. ASSUMPTIONS

The unsaturated zone of Yucca Mountain is a complex hydrogeological system involving a number of important processes relating to fluid flow and solute transport. This section highlights the major assumptions made to develop conceptual and numerical models used to describe these processes. A more detailed discussion of these assumptions is given in Section 6 of this report.

1. Fracture networks are assumed to be represented by a continuum for describing flow and transport processes in the unsaturated zone of Yucca Mountain. The appropriateness of this assumption is mainly supported by the existence of dispersed fractures that actively conduct liquid water. This assumption will be further discussed in Section 6.4.2 of this report. No further confirmation is needed for this assumption.

2. It is assumed that van Genuchten (1980, pp. 892–893) relations, originally developed for porous media, can be used as constitutive relations for liquid flow in the active fracture continuum. Not all connected fractures are active in conducting liquid water in the unsaturated zone of Yucca Mountain. The active fracture continuum consists of fractures that actively conduct liquid water. This assumption results from the use of porous-medium equivalence for describing flow and transport in fractures. A further discussion of this assumption is given in Section 6.4.4 of this report. No further confirmation is needed for this assumption.

3. It is assumed that liquid-water flow in the unsaturated zone of Yucca Mountain is in steady state. As indicated in Wang and Narasimhan (1993, pp. 354–361), the transient behavior of infiltration from the ground surface of the mountain is filtered out because of the damping effects of the near-surface Paintbrush nonwelded unit. A further discussion of this assumption is given in Section 6.1.6. No further confirmation is needed for the assumption.

4. It is also assumed that lateral flow is insignificant within the PTn unit. The early conceptual model of Yucca Mountain (Montazer and Wilson 1984, pp. 45–47) hypothesized that significant lateral flow occurs within the PTn unit, caused by the capillary barrier effect. The recent modeling studies (Ritcey and Wu 1999, pp. 262–268; Bodvarsson et al. 1999, p. 11) indicated that lateral flow in the PTn is reduced with increasing infiltration rate, and the lateral flow is significant only when infiltration rates are far lower than the current estimated values. No further confirmation is needed for the assumption.

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6. ANALYSIS/MODEL

In this section, we discuss the conceptual model and numerical methods used to describe flow and transport processes in the unsaturated zone of Yucca Mountain. These processes are closely related to the hydrogeologic features of the unsaturated zone, which consists of heterogeneous volcanic rocks. These rocks have been welded and fractured to varying degrees, and are divided into hydrogeologic units (Montazer and Wilson 1984, pp. 9–20) based roughly on the degree of welding. Beginning from the land surface, they are the Tiva Canyon welded (TCw), the Paintbrush nonwelded (PTn), the Topopah Spring welded (TSw), the Calico Hills nonwelded (CHn), and the Crater Flat undifferentiated (CFu) hydrogeologic units (Figure 1). The welded units typically have low matrix porosities and high fracture densities, whereas the nonwelded units have relatively high matrix porosities and low fracture densities (Montazer and Wilson 1984, pp. 8-9). Water in the unsaturated zone moving downward through these units is considered to be partitioned between fractures ("fracture flow") and the rock matrix ("matrix flow"), as described subsequently in this AMR.

The conceptual model of flow and transport processes is a framework to explain these processes in the unsaturated zone of Yucca Mountain. The current conceptual model is based to a great extent on the ideas originally presented by Montazer and Wilson (1984, pp. 36–49) and has been developed through the evaluation of collected data and the results of modeling studies. A detailed discussion of the conceptual model is presented in Sections 6.1 through 6.3 of this report. Different numerical methods are available for modeling flow and transport in unsaturated fractured rocks. Section 6.4 briefly reviews the methods and provides an assessment of these methods based on the conceptual model and other practical considerations. The active fracture model will also be documented in this section.

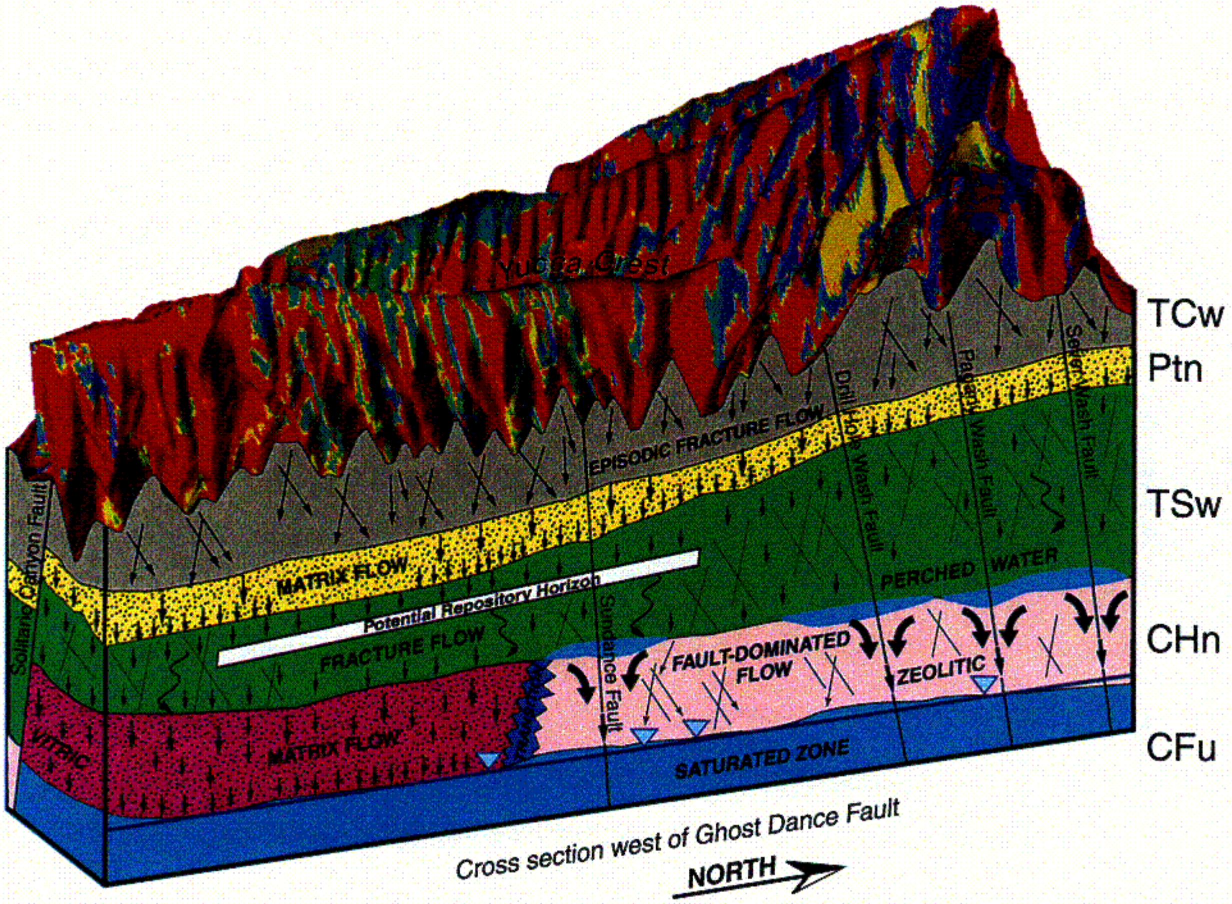

Figure 1. A Simplified Schematic Showing Conceptualized Water Flow through Yucca Mountain. The Blue and Red Colors on the Land Surface Correspond to High and Low Infiltration Rates, respectively, While the Other Colors Correspond to Infiltration Rates in between.

6.1 CONCEPTUAL MODEL OF FLOW

This subsection documents the conceptual model of flow used for modeling flow and transport within the unsaturated zone at Yucca Mountain. The conceptual model is presented by addressing important flow issues and processes.

6.1.1 Infiltration

Infiltration process refers to the penetration of liquid water through the ground surface and to a depth where it cannot longer be withdrawn by evaporation or transpiration by plants. Percolation processes refers to vertical and lateral flow of liquid water within the unsaturated zone. Infiltration is the ultimate source of percolation flux at the repository horizon and provides the water for flow and transport mechanisms that may move radionuclides from the potential repository to the water table. Infiltration is spatially and temporally variable because of the nature of the storm events that supply precipitation (Hevesi et al. 1994, pp. 2520–2529) and variation in soil cover and topography. Infiltration is believed to be high on sideslopes and ridgetops where bedrock crops are exposed, and fracture flow in the bedrock is able to move moisture away from zones of active evaporation (Flint et al. 1994, pp. 2315–2322).

Significant infiltration occurs only every few years. In these years, the amount of infiltration still varies greatly, depending on storm amplitudes, durations, or frequencies. In very wet years, infiltration pulses may infiltrate into Yucca Mountain during a relatively short time period. A more detailed discussion of infiltration at Yucca Mountain will be documented in an AMR describing simulation of net infiltration for modern and potential future climates.

6.1.2 Fracture and Matrix Flow Component

As a result of the relatively high density of interconnected fractures and low matrix permeabilities in the TCw, infiltration pulses are expected to move rapidly through the fracture system with little attenuation relative to travel times in the matrix (Bodvarsson et al. 1999, p. 10). This is partially supported by pneumatic sensors in the TCw showing little attenuation of the barometric signal in monitoring boreholes compared with the barometric signal observed at the land surface (Rousseau et al. 1999, p. 89). In this unit, the gas flow paths are considered to be similar to those of liquid water. The presence of relatively high fractional abundances of ^{36}Cl measured in TCw rock samples from boreholes also supports this conceptual model regarding liquid-water flow. The source of the elevated ("bomb-pulse") ^{36}Cl has been attributed to nuclear testing conducted in the 1950s (Fabryka-Martin et al. 1998, p. 93), and occurrence of ^{36}Cl in the TCw indicates the presence of fast pathways for water flow into and through the unit. A detailed discussion of these data is given in an AMR documenting UZ geochemistry data.

Once the unsaturated flow leaves the TCw and enters the PTn, totally different processes are evident. Because the PTn has relatively high matrix permeabilities and porosities and low fracture densities, the predominant fracture flow in the TCw is expected to convert to dominant matrix flow within the PTn. The uncalibrated properties for the PTn and other units are documented in an AMR describing analysis of hydrologic properties data. Pneumatic data are consistent with the notion that fracturing within the PTn is limited; the pneumatic signal is propagated predominantly through the high-storage matrix, leading to significant attenuation (Ahlers et al. 1999, p. 49). Similarly, much of the water flow occurs in the relatively high-porosity matrix in this unit. As a result, the PTn greatly attenuates infiltration pulses such that liquid-water flow below the PTn is approximately in steady state. This interpretation is consistent with the results of a modeling study of Wang and Narasimhan (1993, pp. 354–361).

Lateral flow is expected to be insignificant within the PTn unit. The early conceptual model of Yucca Mountain (Montazer and Wilson 1984, pp. 45–47) hypothesized that significant lateral flow occurs within the PTn unit, caused by the capillary barrier effect. However, the lateral flow resulting from this mechanism may not be as significant as previously thought, because local heterogeneities and vertical fractures within the PTn unit and at the PTn/TSw and TCw/PTn interfaces may prevent extensive areas of lateral flow from occurring. On the other hand, the recent modeling studies (Ritcey and Wu 1999, pp. 262–268; Bodvarsson et al. 1999, p. 11) indicated that lateral flow in the PTn is reduced with increasing infiltration rate and that lateral flow is significant only when infiltration rates are far lower than the current estimated values. This is because a lower infiltration rate corresponds to a larger capillary pressure gradient in the vertical direction, giving rise to more significant capillary barrier effects. The insignificance of

PTn lateral flow supports the hypothesis that isolated fast flow paths probably carry only a very small amount of water. If a large amount of water flows through a small number of fast flow paths, significant lateral flow in the PTn is needed to provide water for those geological features that cut through the PTn unit and act as fast flow paths. A more detailed discussion on the fast flow paths is given in Section 6.1.7.

Because of its high fracture density and low matrix permeability, water flow in the TSw is considered to be primarily through the fractures. Assuming a unit hydraulic gradient, the matrix percolation rate will be the same as the matrix hydraulic conductivity. Using matrix saturated hydraulic conductivities determined from permeabilities measured in the TSw, the calculated matrix percolation rate is a small fraction of the average infiltration rate currently estimated (Pruess et al. 1999, p. 283). Therefore, the remainder of the flow must be distributed in the fracture network. Calcite-coating data show that most of the deposition is found within the fractures in the welded units (Paces et al. 1998, p. 37), supporting the hypothesis that fracture water flow is a major flow mechanism within TSw. The calcite coating is a signature of liquid-water flow history. Carbon-14 (^{14}C) ages of the perched water bodies below the TSw unit ranges from 3,500 to 11,000 years (Yang et al. 1996, p. 34), again suggesting a fracture-dominated flow within the TSw. The water travel times from the ground surface to the perched water zone are much longer for the liquid water flowing in the matrix (Bandurraga and Bodvarsson 1999, p. 40, Table 3). A detailed discussion on calcite coating and ^{14}C data is given in an AMR describing UZ geochemistry data. Because of the small matrix permeabilities, the perched water bodies would be expected to have much older ages if they result from matrix water flow within the TSw unit.

The occurrence of perched water bodies, reported from a number of boreholes at the lower portion of the TSw and the upper portion of the CHn (Wu et al. 1999a, pp. 159-163), indicates that the layers of the TSw basal vitrophyre and the CHn serve as barriers to vertical flow and cause lateral flow. The main hydrogeologic units below the repository are the CHn and CFu units. Both of these units have vitric and zeolitic components that differ by the degree of hydrothermal alteration (Flint 1998, pp. 29–33). The zeolitic rocks have low matrix permeabilities and some fracture permeability, and therefore a relatively small amount of water may flow through the zeolitic units, with most of the water flowing laterally in perched water bodies and then vertically down faults (Figure 1). On the other hand, similar to the PTn unit, the vitric units have relatively high matrix porosity and permeability, and therefore mostly porous-medium flow predominates. Fracture flow is believed to be limited in these units. A more detailed discussion of the perched water data and conceptual model will be given in an AMR describing UZ flow models and submodels. The relevant hydraulic properties for the different hydrogeologic units are reported in an AMR describing analyses of hydrologic properties data.

6.1.3 Fracture-Matrix Interaction

The transfer of water between fractures and the rock matrix, denoted by fracture-matrix interaction, is likely to be limited within welded units at Yucca Mountain (Bodvarsson et al. 1999, p. 13). The chloride concentration data indicate that perched water was recharged mainly from fracture water, with a small degree of interaction with matrix water (Yang et al. 1996, p. 55). The small degree of interaction between fractures and matrix at locations associated with specific geologic features is also suggested by the presence of bomb-pulse ^{36}Cl (Fabryka-Martin et al. 1998, pp. 93–94) at the potential repository level in the Exploratory Studies Facility (ESF). Studies by Ho (1997, pp. 401–412) evaluate methods of incorporating the conceptual model of fracture-matrix interaction into a dual-permeability model. He shows that the calibration with observed matrix saturation and water-potential data is improved using techniques that reduce the fracture-matrix interaction significantly.

The limitation of fracture-matrix interaction at the Yucca Mountain site is consistent with many other independent laboratory tests as well as theoretical and numerical studies. In a number of laboratory experiments, Glass et al. (1996, pp. 6–7) demonstrated that gravity-driven fingering flow is a common flow mechanism in individual fractures. This mechanism can reduce the wetted area in a single fracture to fractions as low as 0.01 to 0.001 of the total fracture area. However, most of their studies were conducted in analog fractures without interaction with the matrix. Imbibition in the matrix can increase wetted areas of fingering flow patterns in individual fractures, as shown in a numerical study of Abdel-Salam and Chrysikopoulos (1996, pp. 1537–1538). In their study, they investigated unsaturated flow in a quasi-three-dimensional fracture-matrix system (with spatially variable apertures accounting for matrix imbibition). They showed that fingering flow occurs in a fracture, but matrix imbibition will reduce the degree of fingering. Therefore, while fingering flow in individual fractures is an important mechanism for reducing fracture-matrix interaction, its effects may not be as significant as shown in individual fracture experiments without incorporating matrix imbibition.

In a theoretical study, Wang and Narasimhan (1993, pp. 329–335) indicated that the wetted area in a fracture under unsaturated flow conditions is generally smaller than the geometric interface area between fractures and matrix, even when fingering flow does not occur. This results from the consideration that liquid water in an unsaturated fracture occurs as saturated segments that cover a portion of the fracture-matrix interface area. On the other hand, in a recent laboratory experiment study, Tokunaga and Wan (1997, pp. 1287–1295) demonstrated that water film flow could be important in unsaturated fractures. However, note that in their experiments, water film flow becomes important only when the matrix is nearly saturated and water flow occurs from matrix to fractures, as indicated by the conditions of their experiment. Therefore, at this point, we can hypothesize that liquid water generally exists as saturated segments around contact points in unsaturated fractures. The distribution of liquid water in this form will reduce the fracture-matrix interaction (as compared to the case in which the whole geometric interface area is considered to contribute to flow and transport between fractures and matrix).

Liu et al. (1998, p. 2645) suggested that in unsaturated, fractured rocks, fingering flow occurs at both a single fracture scale and a connected fracture-network scale. This is supported in a study of Kwicklis and Healy (1993, pp. 4097–4099). They used numerical simulations to investigate liquid water flow in a simple, unsaturated fracture network and found that a large portion of the connected fracture network played no role in conducting the flow when the fractures do not have uniform apertures. The fingering flow at a network scale has important effects on large-scale flow and transport, and significantly contributes to the reduction of fracture-matrix interaction.

Studies also showed that fracture coating might have important effects on fracture-matrix interaction. Thoma et al. (1992, pp. 1357–1367) performed experiments on actual coated and uncoated tuff fractures and observed that the low-permeability coatings inhibited matrix imbibition considerably. In contrast, fracture coatings may in some cases increase the fracture-matrix interaction when microfractures develop in the coatings (Sharp et al. 1996, p. 1331). Therefore, fracture coating may or may not result in fracture-matrix interaction reduction. Coating effects are not considered in modeling flow and transport in the UZ at Yucca Mountain.

Although several mechanisms exist for limiting fracture-matrix interaction in the UZ, as discussed above, fingering flow at a fracture network scale is considered to be the key mechanism. A newly developed active fracture model based on this mechanism (Liu et al. 1998, pp. 2633–2646) is used for modeling fracture-matrix interaction. This model is documented in Section 6.4.5 of this report.

6.1.4 Perched Water

Perched water is the groundwater in saturated zones that are above or not directly connected to the static water table (Freeze and Cherry, 1979, p. 45). It may occur when large permeability differences exist between geologic units. Perched water zones at Yucca Mountain were reported from a number of boreholes at the lower portion of the TSw and the upper portion of the CHn. The field tests indicated that perched water zones with very different water volumes exist at Yucca Mountain (Bodvarsson et al. 1999, p. 14; Wu et al. 1999a, pp. 159–163). A more detailed discussion on the conceptual models of perched water and analyses of the perched water data will be given in an AMR describing UZ flow models and submodels.

The presence of perched water has important implications for the travel times and flow paths of water through the UZ at Yucca Mountain. First, perched water ^{14}C data indicated that apparent age estimates of perched water bodies range from approximately 3,500 to 11,000 years (Yang et al. 1996, p. 34), suggesting dominant fracture flow in the TSw unit. Second, the occurrence of perched water bodies indicates that the layers of the TSw basal vitrophyre and the CHn serve as barriers to vertical flow and cause lateral flow. Although the vitrophyre is extensively fractured, many of the fractures have been filled with zeolitic materials that impede flow. Portions of the Calico Hills formation have been extensively altered to zeolites, creating the perched water bodies observed within this unit (Bodvarsson et al. 1999, pp. 14–15).

6.1.5 Effects of Major Faults

Numerous strike-slip and normal faults with varying amounts of displacement exist at Yucca Mountain. It is important to understand how major faults affect the flow processes in the UZ at Yucca Mountain.

A fault can act as a fast-flow conduit for vertical liquid-water flow. In this case, transient liquid-water flow may occur within the fault as a result of temporally variable infiltration. Note that major faults cut through the PTn, and the damping effect of the PTn is significantly reduced. This is supported by the correlation of observed "bomb-pulse" ^{36}Cl data and localized geologic features at depth in the UZ at Yucca Mountain (Fabryka-Martin et al. 1998, pp. 93–94). However, if occurring, this transient flow along the major faults is expected to carry only a small amount of water and may not be a significant liquid-flow mechanism for the UZ at Yucca Mountain, as discussed in section 6.1.7. Especially, because the current infiltration model does not support the focusing infiltration mechanism, it is reasonable to assume that recharge through alluvial channels and the associated faults and other potential fast pathways above the potential repository is minimal compared to the overall recharge flux. Note that faults intercepting the perched water bodies, however, can correspond to significant vertical liquid-water flow (see Section 6.1.4).

A fault can also act as a barrier for lateral liquid-water flow. Where a fault zone is highly fractured, the corresponding coarse openings will create a capillary barrier for lateral flow. On the other hand, a fault can displace the surrounding geologic units such that a unit with low permeability faces one with relatively high permeability in a fault zone. In this case, the fault will act as a permeability barrier to the lateral flow within the units with relatively high permeability. Montazer and Wilson (1984, p. 20) conceptualized that permeability would vary along faults, with higher permeability in the brittle, welded units and lower permeability in the nonwelded units where gouge or sealing material may be produced. Whereas a fault sealed with gouge or other fine-grained material would have much higher capillary sections, it will also have low permeability, retarding the movement of liquid water.

In summary, because lateral flow is hypothesized to be insignificant above the repository and significant focusing infiltration near faults may not occur (Section 6.1.7) faults are not considered to contribute significantly to the percolation pattern from the surface to the repository level. Below the repository, low-permeability layers in the CHn channel some flow to faults that act as conduits to the water table. However, the effects of the major faults on gas flow within the UZ are likely to be significant. A more detailed discussion of gas flow processes is given in Section 6.1.8.

6.1.6 Transient Flow

Flow in the UZ is time dependent or transient, mainly resulting from the temporal variation in the infiltration flux at the surface. The temporal variation of the infiltration may be approximated as occurring over short intervals characterized by changes in weather, resulting in episodic transient flows, or over much longer time periods corresponding to climate change.

However, as discussed in Section 6.1.2, the PTn greatly attenuates episodic infiltration pulses such that liquid-water flow below the PTn is considered to be approximately in steady state. This is supported by the modeling study of Wang and Narasimhan (1993, pp. 354–361). The attenuation is a result of matrix flow in the PTn and the relatively large storage that mainly results from the relatively low matrix saturation in this unit. On the other hand, longer-term climate change has a more pronounced influence on flow pattern within the mountain than episodic infiltration and ultimately impacts the entire flow field in the UZ (DOE 1998, pp. 3-115 and 3-116). However, previous modeling studies seem to suggest that use of steady-state flow fields is a good approximation for modeling radionuclide transport in the UZ associated with climate changes (DOE 1998, p. 3-116). The reason for this is that the change in flow in the fractures, which dominates the flux in most hydrogeologic units, responds relatively quickly to a change in infiltration (DOE 1998, p.3-116). Thus, it is reasonable to assume flow to be in steady state for modeling liquid-water flow in the UZ.

It is expected that flow through isolated fast flow paths that by-pass the PTn unit may exhibit a strong transient character, for the lack of a significant attenuation mechanism. However, these isolated flow paths are believed to carry only a small amount of water. More discussions of this issue are given in the next subsection.

6.1.7 Focusing Flow and Fast Flow Paths

Depending on geologic conditions and the magnitude of the water flux, focusing of flow leading to fast pathways through the PTn may occur. Few samples obtained from the lower PTn show "bomb-pulse" signatures of ^{36}Cl (Fabryka-Martin et al. 1998, p. 96, Figure 2). They are generally associated with localized fault structures that cut through the PTn. These pathways are possibly responsible for the presence of high levels of ^{36}Cl that have been detected within the TSw at the potential repository horizon. However, because "bomb-pulse" samples are found only at a few locations, because no significant correlation between high matrix saturation and elevated ^{36}Cl have been reported, and because these discrete "fast paths" are assumed to be not associated with large catchment areas involving large volumes of infiltrating water (based on the current infiltration model), such that the overall flow pattern in the UZ is significantly affected, it is expected that these fast flow paths probably carry only a very small amount of water (Liu et al. 1998, p. 2635). This is also supported by the observation that "bomb-pulse" signatures of ^{36}CI were not found in the perched water bodies, and post-bomb tritium was detected only in one sample from the perched-water, with 10TU, but not for all the other samples. A detailed discussion on these data is given in an AMR describing UZ geochemistry data.

One may consider the fingering flow through the matrix to be an alternative fast flow mechanism through the PTn. Occurrence of fingering flow has been often reported for unsaturated soils (Yao and Hendricks 1996, p. 20). However, it is unlikely that fingering flow is an important flow mechanism for the tuff matrix, because fingering flow is a gravity-driven phenomenon and cannot occur when capillary forces are dominant (Yao and Hendricks 1996, p. 21). One major difference between soils and tuff matrix at Yucca Mountain is that tuff matrix exhibits much stronger capillarities (Wang and Narasimhan 1993, pp. 374–377), which could significantly reduce the possibility for fingering flow to occur in the tuff matrix compared with soils.

A variety of observations indicate that the fracture water flow paths in the TSw are widely dispersed. Average measured matrix saturations suggest relatively uniform values for most of the units (Flint 1998, pp. 24–30, Figures 5–9), and *in situ* water potential measurements also show little variability within the TSw for different boreholes (Rousseau et al. 1999, pp. 143–151). It was also observed that temperature within the TSw unit is fairly uniform (Bodvarsson et al. 1999, p. 13; Rousseau et al. 1999, pp. 151-161). These observations are consistent with a conceptual model in which fracture flow is dispersed, resulting in relatively uniform conditions within the hydrogeologic units.

6.1.8 Gas Flow Process

Gas flow at Yucca Mountain mainly depends on the characteristics of fracture networks. The fractures are generally much more permeable than the matrix because of both their larger absolute permeability and lower liquid saturation. In the welded units, this is particularly true, but in the PTn, the permeability of the fracture continuum is closer to the matrix continuum, because of lower liquid saturation and larger pore sizes in the PTn matrix. Little data exist on gas flow below the bottom of the TSw, though high liquid saturation and low permeability are likely to significantly reduce gas flow. A discussion of the available gas-flow data and liquid saturation data in the UZ is given in an AMR describing the calibrated properties model. The permeability data are discussed in an AMR describing analysis of hydrologic properties data.

The ambient gas-flow processes occurring at Yucca Mountain include barometric pumping, wind, and density-driven flow. Barometric pumping is the response of subsurface pneumatic pressure to changes in atmospheric pressure. Because this is a transient process, both the permeability and storage of the media affect the subsurface response. In the welded units, this translates into little change in the pneumatic pressure signal with depth (Rousseau et al. 1999, pp. 89–97). In the PTn, however, attenuate and lag the response to barometric pumping between the top and the bottom of the unit. Ahlers et al. (1999, p. 58) showed a close correlation between the PTn thickness and pneumatic response below the PTn. They also showed that faults are fast pathways for gas flow but affect subsurface response only at a relatively local scale (Ahlers et al. 1999, p. 47 and pp. 59-66).

Gas flow occurs under ambient conditions as a result of density- and wind-driven processes (Weeks 1987, pp. 165–170). Density-driven flow occurs in the area of deep topography and is a consequence of the differences between the density of dry air in the atmosphere and wet air in the mountain. The wet air is lighter and rises in response to the pressure exerted by the heavier dry air, causing flow within the mountain from the lower elevations toward the crest. Wind-driven flow occurs because of the higher pressure exerted on the windward side of the mountain and the lower pressure in the lee of the crest. Thus, wind-driven flow will also promote flow toward the crest. Measurement of air-flow in an open borehole near the crest of Yucca Mountain shows that density- and wind-driven flow occurs mainly in the TCw (Thorstenson et al. 1989, p. 262).

6.1.9 Summary and Further Discussions

Based on the discussions of flow issues and processes in the UZ (Sections 6.1.1 through 6.1.8), we have constructed a conceptual model of flow in the UZ. Infiltration is mainly characterized by highly spatial and temporal variabilities. Infiltration pulses move rapidly through the fractures in the TCw unit with little attenuation by the matrix. Because of the expected attenuation effects of the PTn unit, the liquid-water flow processes below this unit are considered to be approximately in steady state, under ambient conditions. Lateral flow in the PTn is considered to be insignificant. Fracture liquid-water flow is dominant in welded units and matrix flow in nonwelded units. Dispersed fractures actively conduct liquid water in the UZ of Yucca Mountain. Isolated, transient, and fast flow paths exist, but are expected to transmit only a small amount of liquid water. Fracture-matrix interaction in the welded units is limited. The existence of perched water bodies introduces three-dimensional lateral flow within the unsaturated zone. Major faults do not act as flow paths to significantly alter the percolation pattern from the surface to the repository level. Below the repository, low-permeability layers in the CHn may channel some flow to faults that can act as conduits to the water table.

It is instructive to compare the current conceptual model of flow in the UZ with other conceptual models published in the literature. Since the mid-1980s, the prevailing view of the UZ at Yucca Mountain has been that under ambient conditions, water flow mainly occurs through the rock matrix even in the welded, densely fractured TSw unit (Wang and Narasimhan 1993, pp. 327-339; Peters and Klavetter 1988, pp. 416-430; Nitao and Buscheck 1991, pp. 2099–2112). Based on capillary theory, it was believed that under unsaturated conditions, liquid water would essentially be excluded from fractures because of strong capillarity in the matrix. However, with more and more data available for characterizing the site, it has become evident that unsaturated flow in the welded units is primarily through the fractures, as discussed in Section 6.1.2 of this report.

While the current conceptual model is based to a great extent on the model originally presented by Montazer and Wilson (1984, pp. 36–49), the major differences between these two models are the roles of the PTn unit and structural features, or faults, in conducting liquid water through the UZ. Montazer and Wilson (1984, pp. 50–51) hypothesized that the combination of dipping beds, permeability layering, and capillary-barrier effects results in significant lateral flow within the PTn toward the bounding structural features. Most of the infiltrated water is transmitted downward to the water table along structural features (Montazer and Wilson 1984, p. 51). As discussed in Sections 6.1.2, 6.1.5 and 6.1.7, more recent studies indicate that lateral flow in the PTn may not be as significant as previously thought, and faults are not likely to act as flow paths to significantly alter the flow pattern in the UZ.

In a recent study, Pruess (1999, pp. 1040–1051) proposed a conceptual model for flow in the UZ. While the details of his conceptual model can be found in Pruess (1999, pp. 1039–1050), key elements of the model can be summarized as follows (Pruess 1999, p. 1041):

1. Most of the water flow in thick unsaturated zones of fractured rock proceeds by way of episodic, transient, and localized flow through fractures.

2. Liquid-water flow can remain localized even in the presence of dispersive effects that would tend to cause lateral spreading.

3. Several mechanisms combine to severely reduce the effects of matrix imbibition.

While both the model of Pruess (1999, pp. 1040–1051) and the current conceptual model consider the fracture-matrix interaction to be limited in the UZ and only a portion of fractures to be active in conducting liquid water, they are different in their description of the spatial distribution and time-dependent character of fracture flow. The former hypothesizes that fracture flow paths in unsaturated, fractured rocks are sparse (Pruess 1999, p. 1049) and transient (Pruess 1999, p. 1041). As discussed in Sections 6.1.2, 6.1.6, and 6.1.7, the current conceptual model hypothesizes that liquid-water flow below the PTn unit is approximately in steady state, and fracture flow paths are widely dispersed.

6.2 CONCEPTUAL MODEL OF TRANSPORT

This subsection documents the conceptual model used for modeling transport within the UZ of Yucca Mountain. The conceptual model is presented by addressing important transport issues and processes. Note that transport is closely tied to flow processes, because water is considered to be the principal medium in which solutes are transported through the UZ.

6.2.1 Advective Transport

Advective transport (advection) refers to the movement of dissolved or colloidal materials within the bulk flow of fluid (Fetter 1993, p. 47). Transport is strongly related to liquid water flow through advection, and advective transport pathways coincide with flow pathways discussed in Section 6.1. In welded units, advection through fractures is expected to dominate transport behavior, mainly because liquid water largely flows through fracture networks in these units. Advection is also an important mechanism for transport between fractures and matrix, especially at interfaces between nonwelded and welded units. At these interfaces, transitions occur between dominant fracture flow and dominant matrix flow. Liquid-water flow paths below the potential repository are critical to potential radionuclide transport resulting from advection. Perched water results in lateral transport of the radionuclides. Dominant fracture flow in the zeolitic components of the CHn provides relatively short travel times for transport to the water table, whereas the dominant matrix flow in the vitric components provides much longer travel times.

6.2.2 Matrix Diffusion

Matrix diffusion refers to solute transport from fracture networks into the surrounding matrix blocks resulting from molecular diffusion (Neretnieks 1993, pp. 47–48). Mass transfer between fractures and the tuff matrix may play an important role in transport within Yucca Mountain. Because flow velocity in the matrix is much slower than in fractures, transfer of radionuclides from fractures to the matrix can significantly retard the overall transport of radionuclides to the water table. The transfer can result from advection, dispersion, and diffusion processes. Where fracture flow is dominant, the advection from fractures to the matrix may not be important, because only a relatively small amount of water flows into the matrix, with the rest flowing through fractures. In this case, matrix diffusion may be a major mechanism for mass transfer between fractures and the matrix. On the other hand, the diffusion process in the matrix is more important than dispersion due to the slow pore velocity. Therefore, diffusion is probably the most important physical process in the matrix, which contributes to the retardation of radionuclide transport when fracture flow is dominant.

The significance of matrix diffusion primarily depends on such factors as the effective contact area between fracture and matrix, the effective molecular diffusion coefficient, and the characteristics of fracture networks. Fracture-matrix interaction is expected to be limited in the welded units mainly because of fingering flow in fractures, giving rise to a much smaller fracture-matrix interfacial area being available for matrix diffusion than the geometric contact area between fractures and matrix (see Section 6.1.2 of this report). This can considerably reduce the retardation effect of matrix diffusion (Millington and Quirk 1961, pp. 1200-1207). The effective molecular diffusion coefficient is defined as a product of the free water diffusion coefficient, which is a strong function of solute or radionuclide type, and a factor considering the effects of the unsaturated matrix on diffusion. For a given solute type, the effective molecular diffusion coefficient is mainly dependent on the volumetric water content (Conca and Wright 1990, p. 1055). For rocks in the UZ, the water content is relatively uniform spatially (Flint 1998, pp. 24-30, Figures 5-9). Hence, it is reasonable to assume that the effective matrix diffusion coefficient primarily depends on the solute type for the UZ. In general, matrix diffusion can be an important retardation mechanism for a solute with a relatively large molecular diffusion coefficient, but becomes insignificant when the diffusion coefficient is rather small. Matrix diffusion is also affected by characteristics of fracture networks. As discussed in Section 6.4, only a portion of fractures is active in conducting liquid water in the UZ. The inactive and relatively dry fractures could serve as barriers for flow and transport, including matrix diffusion, between matrix blocks separated by these fractures. A further discussion of this mechanism and its effects on transport will be given in an AMR describing the radionuclide transport model under ambient conditions.

6.2.3 Fracture and Matrix Sorption

Sorption is an important process involved in reactive transport. Sorption refers to a combination of chemical interactions between dissolved solutes and the solid phases (immobile rock matrix or colloids) (Fetter 1993, p. 117). The strength of the sorptive behavior is a function of chemical element, the rock type involved in the interaction, and the geochemical conditions of the water contacting the rock (Domenico and Schwartz 1990, pp. 440–443). Sorption, for example, can act to retard the movement of radionuclides in the groundwater. Reactive chemicals, which are strongly sorbed to rock matrix, are relatively immobile. On the other hand, sorptive interactions may enhance solute transport if the aqueous species sorbs to colloids (Fetter 1993, pp. 149–150). (Colloid–facilitated transport will be discussed in Section 6.2.4).

The importance of sorption in the different rock types is not only a function of the sorptive strength, but also the degree of exposure that solutes have with the rock matrix during transport through the UZ. Zeolitic tuff generally has a larger sorptive strength than vitric tuff, but is a relatively small matrix flow component because of its low matrix permeability (DOE 1998, p. 3-118). Sorption in the zeolitic tuff thus may not be able to effectively retard solute transport with small molecular diffusion coefficients, corresponding to insignificant matrix diffusion. (Transport properties will be reported in an AMR describing UZ/SZ transport properties data.)

The surfaces of fractures, often lined with minerals that differ from the bulk of the rock matrix, may be capable of sorbing many of the radionuclides that may be released from the potential repository (Triay et al. 1997, p. 173). However, characterizing distributions of the fracture-lining minerals and sorptive interactions with these minerals has been limited. Also, the fracture minerals have a relatively small volume and surface area. For these reasons, a conservative assumption in modeling radionuclide transport is that no sorptive interaction with fracture surfaces occurs and that sorptive interactions are only possible for radionuclides in matrix blocks.

Numerous rock-water chemical interactions may influence radionuclide transport. Sorption, representing the combination of these interactions, is characterized by a "sorption" or distribution coefficient (K_d). In general, for a given radionuclide and rock type, this coefficient is not a constant, but depends on the temporally and spatially varied chemical composition of both the aqueous and solid phases (Domenico and Schwartz 1990, pp. 442–443). The latter affects underlying interactions. As a conservative approach to model radionuclide transport through the UZ, a minimum bound for K_d can be used. The minimum K_d represents the smallest reasonable ratio of radionuclides attached to the solid phase versus the aqueous phase. The determination of K_d values for different hydrogeologic units is described in an AMR documenting UZ/SZ transport properties.

6.2.4 Colloid–Facilitated Transport

Radionuclide transport in the UZ at Yucca Mountain may be facilitated by colloidal transport processes. Colloids are particles that are small enough to become suspended (and thus transportable) in a liquid (Fetter 1993, p. 149). They can interact with radionuclides through sorption mechanisms. Unlike sorption of radionuclides to the rock matrix, however, radionuclides sorbed on colloids are potentially mobile. Therefore, colloids can facilitate radionuclide transport through the UZ at a faster rate than the aqueous phase alone (de Marsily 1986, pp. 270–271). Another form of colloidal movement occurs when the radionuclide is an integral component of the colloid structure. In this case, the radionuclide is irreversibly bound to the colloid (DOE 1998, p. 3-105).

The colloid-facilitated transport is controlled by several processes, including advection of colloids, matrix diffusion and dispersion of colloids, sorption of radionuclides on colloids, radioactive decay of radionuclides, and filtration of colloid particles. Advective radionuclide transport paths coincide with liquid-water flow paths below the repository. The advective transport through fractures is enhanced by reduced matrix diffusion and matrix sorption. Colloid particles themselves are not expected to experience any significant matrix diffusion because of the very low diffusion coefficients associated with colloids. Colloids may not be able to move through some of the rock matrix, particularly the welded and zeolitic rock types, because of the colloid size relative to the matrix pore size. However, movement through the more permeable nonwelded vitric rock in the Calico Hills may be possible. The restriction of matrix particle size on movement of colloid particles is the filtration process (de Marsily 1986, pp. 271–272). Obviously, the colloid-facilitated transport becomes a more important transport mechanism for radionuclides that strongly sorb.

6.2.5 Other Transport Issues and Processes

Radioactive decay is a process that affects the concentration of radionuclides during transport through the UZ. For simple decay, radionuclide concentration decreases exponentially with time (de Marsily 1986, p. 265), creating stable decay products. Chain-decay adds another layer of complexity because of the ingrowth of new radionuclides created from the decay of a parent radionuclide. One aspect of potential significance with respect to chain-decay is that daughter products may have significantly different sorption behavior than the parent radionuclide, therefore exhibiting different transport behavior.

Dispersion is a transport mechanism caused by localized variations in flow velocity (de Marsily 1986, pp. 234–235; p. 244). However, it is not expected to play an important role in the UZ transport (CRWMS M&O 1998, Section 7.2.3). An important reason that dispersion is secondary is the explicitly modeled variations in transport velocity caused by the fracture–matrix system. (A further discussion of this issue will be presented in Section 6.4.3 of this report.) In the rock matrix, dispersion is also considered to be minor compared with diffusion because of the low pore velocity in the matrix. Dispersive flux is propotional to pore velocity (de Marsily 1986, pp. 236–238).

The presence of perched water may serve as a mechanism to dilute liquid-phase solute concentrations in the UZ. In the TSw unit above perched water, solutes are expected to be carried primarily by many flow channels within active fractures. Once they arrive at perched water, these solutes would be mixed with water in the perched water body, resulting in a decrease in chemical concentrations. The degree of dilution depends on the residence time of the solutes in the perched water: longer residence time corresponds to a larger degree of mixing within the perched water and therefore a larger degree of dilution. The relevant observations and modeling studies seem to indicate that a large degree of mixing occurs in the perched water (Sonnenthal and Bodvarsson 1999, p. 118, p. 151). Sonnenthal and Bodvarsson (1999, p. 118) observed that chloride concentrations in water samples collected during hydraulic tests in the perched water bodies are not very variable because the water is probably well mixed. Their modeling exercise also showed that perched water compositions are best matched by a mixture of Pleistocene age water with variable amounts of modern water (Sonnenthal and Bodvarsson 1999, p. 151).

6.2.6 Summary and Further Discussions

Based on the discussions of transport issues and processes for the UZ (Sections 6.2.1 through 6.2.5), we have constructed a conceptual model of transport in the UZ that can be summarized as follows. Advective transport pathways coincide with flow pathways. Matrix diffusion is a major mechanism for mass transfer between fractures and matrix, and is expected to contribute to the retardation of the radionuclide transport when fracture flow is dominant. Sorption may retard the movement of radionuclides in the UZ, but this retardation is limited by the reduction of fracture-matrix interfacial area resulting from fingering flow in fractures. However, sorptive interactions may enhance radionuclide transport if the aqueous species sorbs to colloids that subsequently may be transported through the UZ. Dispersion is not expected to be a major transport mechanism in the UZ.

It is useful to emphasize that flow is a major driving force for transport. As a result, the conceptual model of transport in the UZ is closely tied to the conceptual model of flow. Alternative conceptual models of flow give rise to different transport behavior from that discussed above. If the liquid-water flow primarily occurs in the matrix—as hypothesized by Wang and Narasimhan (1993, pp. 327-339), Peters and Klavetter (1988, pp. 416–430) and Nitao and Buscheck (1991, pp. 2099-2112)— matrix diffusion will be insignificant for UZ transport, and colloid-facilitated transport may not need to be considered given that it mainly occurs in fractures. In contrast, if most liquid-water flows through structural features (Montazar and Wilson 1984, p. 51) or sparse flow paths (Pruess 1999, pp. 1040–1051), transport will be primarily determined by flow in fractures and the effects of the matrix, such as matrix diffusion and matrix sorption, become insignificant. However, as discussed in Section 6.1.9 of this report, liquid-water flow in the UZ is considered more likely to be consistent with the current conceptual model of flow rather than those proposed by these authors.

6.3 COUPLED PROCESSES: EFFECTS ON FLOW AND TRANSPORT

If the Yucca Mountain site is determined to be suitable and is licensed, the DOE is planning to emplace, in a geologic repository at the site, radioactive wastes that will emit a significant amount of radioactive decay heat. This heat will influence hydrologic, mechanical, and chemical conditions in both the near field (drift-scale) and far field (mountain-scale). This subsection discusses the effects of the corresponding coupled processes, including thermo-hydrologic (TH), thermo-mechanical (TM), and thermal-chemical (TC) processes, on flow and transport within the UZ at Yucca Mountain. Note that TH, TM and TC processes are still coupled among themselves, although they are discussed separately (for reasons of simplicity) in this subsection.

6.3.1 TH Processes

The expected TH response of the unsaturated, fractured tuff to potential radioactive decay heat involves a number of key processes (Buscheck and Nitao 1993, pp. 418-448; Tsang and Birkholzer 1999, pp. 389–390). As the formation temperatures rise around waste packages, pore water boils and vaporizes. Most of the vapor generated moves into the fractures, where it becomes highly mobile and is driven with the gas-pressure gradient and gas-density differences above and away from the drifts. The heated dryout zone can prevent the infiltrating water from moving down through the potential repository horizon, resulting in a drop in the water flux at the potential repository depth. When the vapor encounters cooler rock above and below the potential repository, it would condense, and the local fracture saturation would build up. Part of the condensate may then imbibe into the matrix, where it is subject to a very strong capillary pressure gradient toward the heat sources, giving rise to a reflux of liquid water to the repository. Condensate also will remain in the fractures and becomes mobile. Some fraction of the condensate in the fractures may flow back toward the boiling zone; however, as capillary forces are relatively weak in the fractures, a substantial amount of liquid may drain by gravity. The gravity-driven reflux in fractures is characterized by fingering flow at different scales. The stronger the vapor flux away from the drifts and the reflux towards the drifts, the more obvious will be the 'heat pipe' signature in the temperature fields (namely, a small temperature gradient due to the persistence of liquid-vapor counterflow). Where heat pipe conditions exist, the temperature remains at the nominal boiling point. Eventually, the heat output is decreased and becomes small enough not to affect the liquid flow field, so that the flow field returns to a steady state.

Thermal hydrology drives processes at two physical scales. At the drift scale, flow and transport is affected by decay-heated characteristics from each of the individual waste packages in an emplacement drift. The thermodynamic environment within the emplacement drift is related to the drift and waste package geometry, waste package spacing and sequencing, drift-to-drift spacing, and individual waste-package heat outputs. Variability of heat output from waste packages could result in large variabilities in dryout, rewetting, and liquid-phase flux along drifts. A cooler waste package may receive more reflux, corresponding to an earlier rewetting time. Water may also flow (drain) preferentially downward through connecting fractures between emplacement drifts (Kneafsey and Pruess 1998, p. 263, Figure 2). At the potential repository edges, the surrounding rocks receive a smaller amount of heat than those farther from the edges within the repository horizon. The drifts located near the edges could thus correspond to smaller dryout zones and have earlier rewetting times.

The emplacement of heat-generating wastes in the potential repository will alter large-scale flow and transport processes associated with the mountain scale. Heat-driven features at this scale potentially include the development of large-scale, gas-phase, buoyant convection cells and thermally altered liquid-phase flow fields both above and below the repository. The latter may be especially important for radioactive transport because such transport occurs primarily through the liquid phase (Haukwa et al. 1999, p. 227). Heating can generally increase the liquid flow into the repository (Haukwa et al. 1999, pp. 247–248). The significance of TH effects on radionuclide transport is also largely determined by the duration of the thermal perturbation compared with the waste package lifetimes. If the perturbation becomes insignificant before most packages fail and release significant amounts of radionuclides, the TH processes are expected to have a minor effect on radionuclide transport (Robinson et al. 1998, p. 157).

6.3.2 TM Processes

The heat-transfer processes result in elevated temperatures of the host rock surrounding the potential repository and therefore mechanically change physical properties of the rock within the UZ (Wang et al 1998, pp. 108–110). Expansion of the rock matrix caused by heating will create stress in the rock and induce changes in the fracture apertures. These changes can affect the amount of flow that occurs in the fractures and subsequently through the entire system. These hydrologic changes can, in turn, affect thermal behavior, which governs the mechanical changes of the rock.

Thermal expansion of the matrix surrounding the drifts will tend to "close" fractures and reduce fracture aperture and permeability while increasing capillary forces. However, nonuniform deformation of heterogeneous matrix rock blocks will promote sliding or relative movement along two adjacent matrix block surfaces, which may lead to an increase in fracture permeability. In general, the reduction of fracture apertures could limit the development of gas-phase transport, including vapor transport, near the drift. This effect could limit the growth and extent of the dryout zone surrounding the drift. Compared with the situation without TM effects, liquid fracture flow may or may not be reduced. On the one hand, reduction of fracture permeability can reduce fracture liquid-water flow. On the other hand, a smaller fracture air-entry pressure causes more liquid to be retained in fractures because of higher capillary suction, giving rise to relatively large relative permeability for a fracture network. However, reduction of the dryout zone is expected to result in relatively early rewetting times for waste packages. During the cooling phase, the fracture apertures near the drifts would generally increase. For rock relatively far away from the repository, TM processes are expected to have a minor effect on the hydrologic properties.

A key concern in modeling mechanical effects on flow and transport is how flow and transport properties are modified by rock deformation. The following correlations may be used in solving the governing equations of flow and transport:

$$\phi = \phi(\sigma_{ij}) \tag{Eq. 1}$$

$$k = k(\phi) \tag{Eq. 2}$$

$$P_c = P_{c,I} \frac{(k/\phi)_I^{1/2}}{(k/\phi)^{1/2}} \tag{Eq. 3}$$

where ϕ (-) is the effective porosity and $k(m^2)$ is the absolute permeability of fractures or matrix, σ_{ij} (Pa) are the components of the total stress tensor, P_c (Pa) is capillary pressure, and subscript I denotes the initial values, corresponding to ambient conditions. Note that the capillary pressure is modified using the Leverett (1941, pp. 157-169) relation. Considering that there is a large degree of uncertainty in modeling the TM processes, the effects of temperature change on surface tension are (for simplicity's sake) not considered in Equation 3.

6.3.3 Thermo-Chemical Processes

Chemical effects in response to a high thermal load in the potential repository can alter material hydrologic properties (Hardin 1998, p. 2-3). Above the potential repository level, the temperature is projected to be sufficiently high to vaporize the water, resulting in precipitation of minerals in fractures. The condensate, being out of equilibrium with the rock, can dissolve mineral phases from the wall of fractures and flow back to zones where precipitation occurs. Below the potential repository, the processes are not completely the same because the liquid within the fractures, under the influence of gravity, can migrate away from the heat source and leave the two-phase flow system. This dissolution of minerals at one point in the fracture network and their redeposition at another could lead to the formation of a precipitate cap over the potential repository. In the precipitate cap, porosities and permeabilities of fractures and portions of matrix near the fractures will be reduced. The significance of this reduction depends on the abundance of readily dissolved fracture-lining minerals, and the dissolution and precipitation rates for the relevant minerals (Hardin 1998, p. 2-8). When the thermal perturbation is considerably decreased, the cap may start to be dissolved by water from ambient percolation. Since the process of dissolution is much slower than the process of precipitation, the existence of the cap may exist virtually permanently after the thermal perturbation. Therefore, these changes will influence the flow field not only while the thermal process is active, but afterward (Hardin 1998, p. 2-2).

6.4 NUMERICAL APPROACHES

In this section, we briefly review the currently available numerical approaches that can be used for modeling flow and transport in unsaturated fractured rocks, followed by a discussion of the appropriateness of these approaches for use in the UZ flow and transport model and other relevant issues.

6.4.1 Available Numerical Schemes

A variety of numerical approaches have been proposed in the literature to deal with flow and transport processes in fractured media at the field scale. When classified according to the manner in which fracture networks are treated in the model structure, the approaches fall into one of three groups: continuum approaches, discrete fracture-network approaches, and other approaches. Excellent reviews on these approaches, which have been developed and used in different fields (including oil-reservoir engineering, groundwater hydrology, geothermal engineering and soil physics), can be found in Bear et al. (1993, pp. 267–320 and 396–428) and the National Research Council (1996, pp. 307–394). We do not intend to give a comprehensive review of all the approaches, but will rather focus on those that can be used for unsaturated, fractured rock.

6.4.1.1 Continuum Approaches

6.4.1.1.1 Basic Physical and Numerical Principles

In continuum approaches, fractures are considered to be sufficiently ubiquitous and distributed in such a manner that they can be described statistically in a meaningful way (Bear et al. 1993, pp. 395–396). The role of individual fractures in fractured media is considered to be similar to that of individual pores in porous media. Therefore, one can describe average fracture properties as macroscopic and those associated with individual fractures as microscopic. Theoretically, the macroscopic scale is related to the so-called Representative Elementary Volume (REV) (Bear et al. 1993, pp. 3-10). A physical property value at a "point" in the fracture or matrix continuum is defined as that averaged over the corresponding REV. When the continuum approaches are valid, the size of a REV must be much larger than the scale of microscopic heterogeneity and much smaller than the scale of whole flow and/or transport domain.

In continuum approaches, connected fractures and rock matrix are viewed as two or more overlapping, interacting continua. In other words, at a "point," two or more continua are considered to co-exist. In this case, the continuum mechanics formulations, such as those used for porous media, can be used to describe flow and transport in each continuum. Coupling of processes between different continua is determined by interaction mechanisms at a subgrid scale.

Depending on the number of continua and methodologies used to treat fracture-matrix interaction, continuum approaches can be further classified as effective-continuum (ECM), dual-continua, and multiple interacting continua (MINC) approaches.

6.4.1.1.2 Effective Continuum Approach (ECM)

In the ECM approach, fractures and rock matrix are replaced with a single effective continuum (Figure 2). In the traditional ECM (Pruess and Tsang 1994, pp. 47–49), nonzero liquid saturation in the fracture does not occur until the matrix is fully saturated, which occurs at the so-called threshold saturation. Composite characteristic curves are constructed which embody matrix behavior when the saturation of the effective continuum is less than the threshold saturation and fracture behavior when the saturation is larger than the threshold saturation. In the generalized ECM (Wu et al. 1999b, p. 194), the concept of threshold saturation is not invoked. Instead, liquid saturation is partitioned into the matrix and fracture in accordance with the principle of local thermodynamic equilibrium, which requires capillary pressure in the matrix and fracture components of a gridblock to be equal. Thus, in the generalized ECM formulation, fracture flow occurs at all saturations, although small fracture flow is computed at low saturations. Note that in each gridblock, ECM also assumes that water in the fractures and matrix have the same chemical concentration and temperature.

The ECM approach provides a substantial simplification for describing flow and transport in fractured porous media, and is computationally efficient in handling a large model grid. However, the assumptions on which ECM is based may break down when long times are needed to reach local equilibrium condition between the fracture and matrix continua. This is especially true for a very tight and low-permeability rock matrix with rapid fracture flow (Wu et al. 1999b, p. 195).

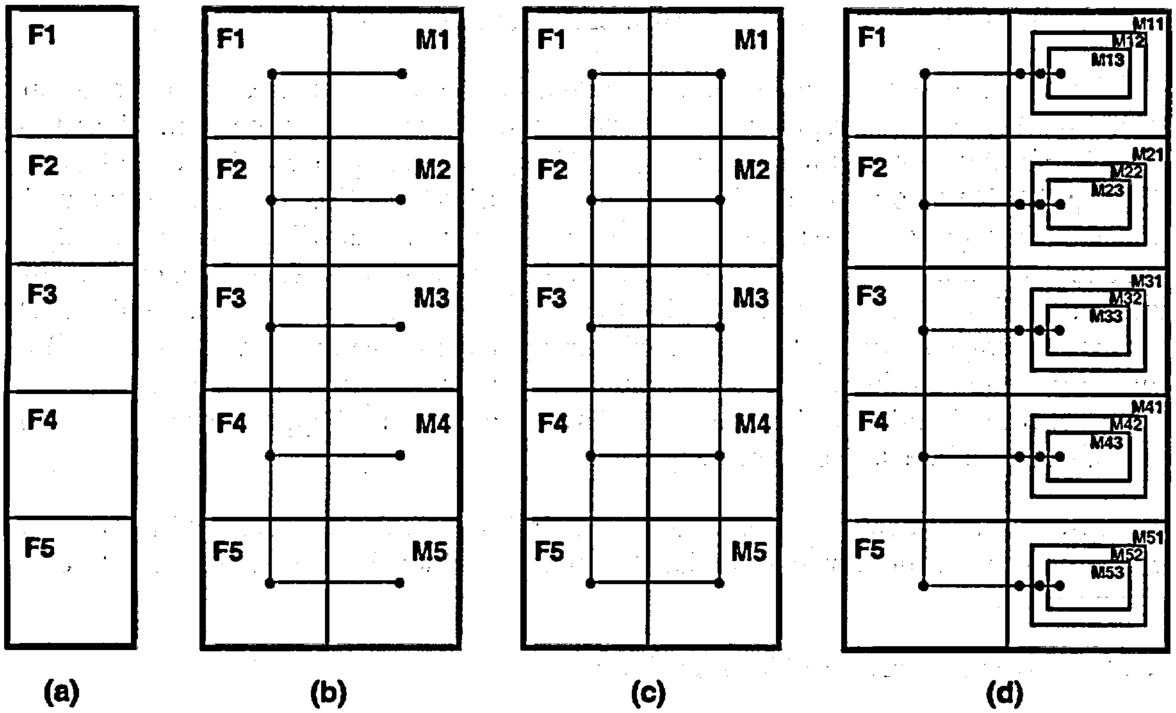

Figure 2. Schematic Diagram of One-Dimensional Column of Gridblock, Modeled as (a) ECM, (b) Dual-Porosity with One Matrix Gridblock, (c) Dual-Permeability with One Matrix Gridblock per Fracture Gridblock, and (d) MINC with 3 Matrix Gridblocks per Fracture Gridblock.

6.4.1.1.3 Dual-Continua Approaches

In dual-continua approaches, fractures and matrix are treated as two separate, yet interacting continua, and each gridblock is subdivided into one fracture block and one matrix block (Figure 2). The fracture-matrix flow and transport are approximated as quasi-steady. This treatment is the numerical equivalent of the Warren and Root formulation (1963, pp. 245-255). If global flow occurs only between fracture gridblocks, the approach is known as a dual-porosity approach, because fractures alone control large-scale fluid flow and the matrix only contributes an additional storage term. If global flow occurs within both fracture and matrix continua, the scheme is known as a dual-permeability approach (Doughty 1999, p. 76).

Compared to ECM, dual-continua approaches can more accurately predict flow and transport, because nonequilibrium is allowed between fracture and matrix continua. The dual-porosity approach is valid only when matrix flow is not important. When both fracture flow and matrix flow are important, the dual-permeability scheme is more accurate. On the other hand, since only one matrix block is used for each gridblock and a quasi-steady fracture-matrix flow assumption is employed, gradients of matrix capillary pressures, temperature, and concentration near a fracture-matrix interface may be poorly predicted using dual-continua schemes. This is especially true during a rapid, transient flow or transport period in a system with large size and low-permeability matrix blocks. Therefore, the dual-continua approach could give rise to poor solutions to fracture-matrix flow for rapid, transient flow and transport. Under steady-state conditions, however, the gradients near the matrix surface become minimal, and the approaches are expected to produce acceptable solutions.

6.4.1.1.4 Multiple Interacting Continua Approach (MINC)

As indicated previously, dual-continua approaches could give rise to poor solutions to fracture-matrix flow for rapid, transient flow and transport. A more general and rigorous approach, multiple interacting continua (MINC), was developed by Pruess and Narasimhan (1985, pp. 14–26) to overcome this limitation. Specifically, MINC is based on the notion that changes in fluid pressures, temperature, and phase compositions will propagate rapidly through the fracture system, while invading the tight matrix blocks slowly. Therefore, changes in matrix conditions will be locally controlled by the distance from the fractures. In the MINC, all fractures are lumped into Continuum #1, all matrix materials within a certain ("small") distance from the fractures are lumped into Continuum #2, matrix materials at larger distance from the fractures become Continuum #3, and so on. Therefore, the MINC approach can be considered as a generalization of the dual-continua approach.

Compared with dual-continua approaches, the MINC approach can more accurately predict flow and transport in fractured media, but has larger computational requirements in both CPU times and storage space.

6.4.1.2 Discrete Fracture-Network Approaches

Discrete fracture-network approaches are based on an assumption that flow and transport behavior can be predicted from knowledge of the fracture geometry and data on hydraulic properties of individual fractures (National Research Council 1996, p. 332). These approaches involve computational generation of synthetic fracture networks and subsequent modeling of flow and transport in each individual fracture. These approaches have been extensively used for single-phase flow and transport, with deterministic, stochastic, artificial, or site-specific fracture networks in two or three dimensions (National Research Council 1996, pp. 333-350). Recently, the same approaches have also been applied to unsaturated conditions (e.g., Kwicklis and Healy 1993, pp. 4091-4102).

While discrete fracture-network approaches are useful as tools for concept evaluation or model-based process studies, they have several limitations. First, the approaches require geometric parameters that may strongly impact flow and transport, such as fracture apertures and conductivity, but typically cannot be well constrained from field observations (Pruess et al. 1999, p. 308). Second, it is difficult to separate the conductive fracture geometry from the nonconductive fracture geometry (National Research Council 1996, p. 350). Third, flow and transport models based on these approaches can be complex and computationally intensive for realistic fracture densities (National Research Council 1996, p. 350). Fourth, so far, the studies based on discrete fracture-network approaches have rarely considered fracture-matrix interaction because of computational complexity (Pruess et al. 1999, p. 308). Fracture-matrix interaction has important effects on flow and transport in unsaturated fractured rocks.

6.4.2 Assessment of Numerical Approaches

Several basic numerical approaches for unsaturated, fractured porous media have been briefly reviewed, and the advantages and limitations of these approaches have also been discussed. It needs to be indicated that several other numerical approaches are also available in the literature (e.g., Clemo and Smith 1997, pp. 1763–1765). These additional approaches, however, can be considered as variations and/or combinations of the basic approaches mentioned above. The appropriateness of the currently available numerical approaches for the UZ flow and transport model depends on several important factors, including flow and transport behavior at the Yucca Mountain site, scale of the problem, data availability, and computational feasibility.

The overall flow and transport behavior in the UZ at Yucca Mountain may be characterized by two important features. The first feature is the coexistence of a few isolated, transient, fast flow paths and relatively uniform flow and transport within fractures. As discussed in Section 6.1.7 of this report, the isolated flow paths only carry a small amount of water and do not significantly contribute to the overall flow and transport patterns in the UZ. Therefore, the dispersed nature of fracture flow should be the critical basis for assessing numerical approaches for fracture flow and transport. This makes continuum approaches reasonable choices for the UZ model. The second feature is the coexistence of matrix-dominant flow and transport in nonwelded units and fracture-dominant flow and transport in welded units. The feature can be easily handled by continuum approaches, but not by other approaches such as a fracture-network model. For example, as previously indicated, studies based on discrete fracture-network approaches have rarely considered fracture-matrix interaction because of computational complexity (Pruess et al. 1999, p. 308). Consideration of this feature is important for correctly simulating flow and transport processes in the UZ of Yucca Mountain.

Scale of the problem is an important factor for assessing the appropriateness of numerical schemes for the UZ flow and transport model. Because continuum approaches are relatively simple and straightforward to implement, they are preferred for most applications that are encountered in practice (National Research Council 1996, p. 331). There are estimated to be on the order of 10^9 fractures at Yucca Mountain (Doughty 1999, p. 77). It is practically impossible to construct and calibrate a discrete fracture network site-scale model with so many fractures, considering the data availability and computational feasibility.

Based on the above considerations, continuum approaches have been considered to be appropriate for use in the UZ flow and transport model. As a compromise between accuracy and feasibility, the dual-permeability method has become the main modeling approach currently used in the UZ model to simulate water flow, heat transfer, and chemical transport.

6.4.3 Heterogeneity and Parameterization

Heterogeneities exist at different scales within both the fracture and matrix continua in the UZ at Yucca Mountain. Parameterization refers to the use of a number of parameters to represent the heterogeneous distribution. Treatment of subsurface heterogeneity and parameterization are important for modeling flow and transport processes. A geologic-based, deterministic approach, in which an entire model layer is assigned uniform properties, is mainly used for characterizing subsurface heterogeneity and modeling flow and transport in the UZ of Yucca Mountain.

The geologic-based deterministic approach is based on the following considerations. First, it is generally believed that overall behavior of site-scale flow and transport processes are mainly determined by relatively large-scale heterogeneities associated with the geologic structures of the mountain. Second, the complexity of a heterogeneity model needs to be consistent with the availability of the data. More complicated models introduce larger degrees of uncertainties in rock-property estimates when data are limited. This is because more complicated models generally correspond to larger numbers of variables. Third, the layered approach is also supported by field observations, such as matrix water-saturation distributions. For a given geologic unit, measured matrix saturation distributions are very similar in the different boreholes (Flint 1998, pp. 24–30, Figures 5-9), indicating that matrix flow behavior and effective hydraulic properties should be similar within the unit. Fourth, a flow and transport model based on a layered approach can be relatively easily calibrated with multiple data sets and provides a means to incorporate a significant amount of the available site data. Fifth, it is straightforward to deal with the upscaling issues using inverse modeling when a layered approach is employed. This is because effective parameters can be inferred directly by matching the large-scale simulation results with gridblock-scale observations averaged from small-scale measurements.

6.4.4 Special Issues for Flow and Transport Modeling

In the dual-continua approach, porous-medium equivalence has been used for describing water flow in the fracture continuum (National Research Council 1996, p. 380). Specifically, Darcy's law is used to determine water flux within the fracture continuum, and constitutive relations between relative permeability, capillary pressure, and saturation are employed for modeling water flow. However, the physics of water flow in fracture networks is not exactly the same as that in porous media. Because of the lack of better alternatives, van Genuchten (1980, pp. 892-898) relations, originally developed for porous media, are used as constitutive relations for liquid water flow in the active fracture continuum. The active fracture continuum consists of fractures that actively conduct liquid water and is only a portion of the whole fracture continuum. A further discussion of this issue can be found in Section 6.4.5 of this report.

Gas flow behavior is different from that of liquid water. No data are available to characterize gas relative permeability in the UZ of Yucca Mountain. It is reasonable to expect phase interference to reduce the mobility of the gas phase in both the matrix and the fractures. Indirect evidence of the reduction for gas flow between fractures and the matrix is found in the pneumatic pressure data (Rousseau et al. 1999, pp. 77–110). These data show insignificant attenuation and lag of the pneumatic signal through the TSw, which requires high permeability and/or low porosity. The gas saturation in the fractures is very high, so the relative permeability of the gas phase in the fractures will also be high. The effective porosity for the gas-phase system can be reduced by reducing the mobility (or saturation) of the gas phase in the matrix, which provides a substantial portion of the gas-phase storage in the TSw. The widely used Brooks-Corey relationship for gas relative permeability, k_{rg} (-), is suitable for this problem and is given by (Brooks and Corey 1966, p. 71)

$$k_{rg} = (1 - S_e)^2 \left(1 - S_e^{\frac{2+\lambda}{\lambda}}\right) \qquad \text{(Eq. 4)}$$

where λ (-) is a pore-size distribution parameter and S'_e (-) is effective saturation, given by

$$S'_e = \frac{S - S_r}{S_s - S_r} \qquad \text{(Eq. 5)}$$

where S (-) is liquid saturation, S_r (-) is residual liquid saturation, and S_s (-) is satiated liquid saturation. For the van Genuchten relationship, which is used to describe liquid relative permeability and water potential, pore-size distribution is determined from liquid desaturation data. The van Genuchten pore-size distribution parameters n (-) and m (-) can be related to the Brooks-Corey λ by (van Genuchten 1980, p. 895)

$$\lambda = n - 1 = \frac{m}{1-m} \qquad \text{(Eq. 6)}$$

Substituting Equation 6 into Equation 4 gives

$$k_{rg} = (1 - S'_e)^2 \left(1 - S'^{\frac{2-m}{m}}_e\right) \qquad \text{(Eq. 7)}$$

Equation 7 is used to describe the gas relative permeability in the fractures and matrix, and uses the same m as the liquid relative-permeability and water-potential relationships. Finally, it should be indicated that consideration of the reduction makes calibrated fracture permeabilities more consistent with those determined from air injection tests by LeCain (1997, pp.31-32). Otherwise, the calibrated fracture permeabilities would be unrealistically high given the data showing insignificant attenuation and lag of the pneumatic signal through the TSw. A detailed discussion of calibrated fracture permeabilities is given in an AMR describing the calibrated properties models.

In general, there are two kinds of numerical algorithms for modeling chemical transport in the subsurface. One is the conventional algorithm based on finite-difference and/or finite-element methods. Another is the particle-tracking algorithm. In a particle-tracking algorithm, chemical mass is divided into a large number of particles. Chemical transport is simulated by calculating particle movement, which is determined by velocity fields, dispersion/diffusion coefficients, and fracture-matrix interaction formulations. Compared with the conventional approaches, particle tracking has the following two advantages. First, it can significantly reduce or eliminate numerical dispersion. Numerical dispersion is a common numerical problem for coarse grid simulations of chemical transport problems. It artificially smears concentration fronts in simulations. Second, the particle-tracking algorithms can be computationally more efficient. However, one shortcoming of particle-tracking algorithms is that they can only be used for chemical transport with simple chemical reactions like linear adsorption and decay. The above considerations suggest that particle-tracking algorithms are appropriate for modeling chemical transport with simple reactions, and conventional algorithms are appropriate for transport with complex reactions. Note that both particle tracking and conventional algorithms should yield similar simulation results for transport with simple reactions when numerical dispersion is insignificant. A detailed comparison between the particle-tracking algorithms and conventional algorithms is being considered in a separate AMR.

Although it is generally recognized that dispersion in a fractured medium is physically different from dispersion in a porous medium, the porous medium form of the dispersion tensor is generally used for lack of a more appropriate expression (Bear et al 1993, p. 419). As discussed in Section 6.2.5, the dispersion may not be a major transport mechanism for the UZ of Yucca

Mountain. It physically makes sense. For a dual-continua system, chemical transport is mainly determined by the largest heterogeneity, the difference in properties between the matrix and fracture continua. In this case, heterogeneity in each continuum, resulting in the corresponding macroscopic dispersion process, becomes secondary. Therefore, a more accurate description of the fracture dispersion may not significantly improve the accuracy of transport simulations. This is supported by a tracer transport simulation study on the ESF Alcove 1 test, documented in an AMR describing UZ flow model and submodels. The Alcove 1 modeling study shows that the simulation results are sensitive to matrix diffusion, but not to dispersion in the fracture continuum.

Since radionuclide transport is a transient process, the use of the dual-continua approach may result in some modeling errors for chemical transfer between fractures and the matrix. This is particular true when the chemical transfer occurs only within a portion of matrix close to the fracture-matrix interfaces. Generally, the dual-continua approach may underestimate the chemical concentration gradient at the fracture-matrix interface, and therefore may underestimate chemical transfer from fractures to matrix under certain conditions. This is confirmed by the modeling study of Doughty (1999, pp. 94-95), showing that the dual-continua approach yields shorter travel times than the MINC approach. Note that 1-k and 5-k in Doughty (1999, pp. 94–95) correspond to the dual-permeability (with one matrix continua) and the MINC with 5 matrix continua, respectively (Doughty 1999, pp. 80-82). Since the matrix transport processes correspond to relatively long travel times to the water table compared with those in fractures, the dual-continua approach is expected to give conservative predictions of radionuclide transport in the unsaturated zone.

6.4.5 Active Fracture Model

In a dual-continua approach, the treatment of fracture-matrix interaction is important for accurate modeling of flow and transport. This subsection discusses the active fracture model used in the UZ Flow and Transport Model.

6.4.5.1 Active Fracture Concept

Although a number of mechanisms exist (Section 6.1.3), fingering flow at a fracture network scale is considered to be a key mechanism for limiting fracture-matrix interaction, more important than that at a single fracture scale. We expect that for unsaturated fractured rock the water-flow pattern should be characterized by significant preferential (fingering) flow at a fracture-network scale, because of the large nonlinearity involved in an unsaturated system and heterogeneities of fracture structure at different scales. The active fracture concept is based on the reasoning that as a result of fingering flow, only a portion of fractures in a connected, unsaturated fracture network contribute to liquid water flow, while others are simply by-passed. The portion of the connected fractures that actively conduct water are called *active fractures*. We hypothesize that the number of active fractures in the UZ of Yucca Mountain is small compared to the total number of connected fractures. With this in mind, active fractures, rather than total connected fractures, must be used in numerical models. We further hypothesize that the number of active fractures within a gridblock is large, such that a continuum approach is still valid for describing fracture flow. These hypotheses are consistent with the consideration that flowing fractures in the unsaturated zone are many and highly dispersed.

To use the active fracture concept to model flow and transport in fractures, we treat active fractures as a portion of the "homogeneous" fracture continuum for a given gridblock. It is important to note differences between the active fracture model and the conventional, capillary-equilibrium-based, fracture water distribution model. The latter assumes that liquid water occupies fractures with small apertures first, and then fractures with relatively large apertures as water potential (or water saturation) increases. In contrast, the active fracture model presumes gravity-dominated, nonequilibrium, preferential liquid water flow in fractures, which is expected to be similar to fingering flow in unsaturated porous media. A liquid finger can by-pass a large portion of a porous medium, which does not necessarily correspond to large pores. It is also consistent with the numerical study results of Kwicklis and Healy (1993, pp. 4097–4099), showing that distribution of liquid water in a connected fracture network is not necessarily determined by fracture apertures.

Flow and transport conditions and fractured rock properties should determine the fraction of active fractures in a connected fracture network, f_a. An expression for f_a must satisfy the following conditions: all connected fractures are active ($f_a = 1$) if the system is fully liquid saturated; all fractures are inactive ($f_a = 0$) if the system is at residual saturation; and f_a should be related to water flux in fractures. More fractures are considered to be conducive for a larger water flux (Liu et al. 1998, pp. 2635-2636). The water flux in fractures is also considered to be mainly dependent on fracture saturation because fracture water flow is gravity-dominated. A simple expression for f_a (-) (Liu et al. 1998, pp. 2035-2536) that meets these conditions and includes one parameter only is a power function of effective water saturation in connected fractures, S_e (-):

$$f_a = S_e^{\gamma} \tag{Eq.8}$$

where γ (-) is a positive constant depending on properties of the corresponding fracture network, and the effective water saturation in connected fractures is given by

$$S_e = \frac{S_f - S_r}{1 - S_r} \tag{Eq.9}$$

where S_f(-) is the water saturation of all connected fractures and S_r is the residual fracture saturation. In this study, Equation 8 is used to determine the fraction of active fractures because it is mathematically simple. As discussed below, Equation 8 allows us to treat all the ramifications of the active fracture hypothesis (modified fracture capillarity, relative permeability, and fracture-matrix interaction reduction) in an integrated manner.

Note that f_a may be a very complicated function of fracture-matrix system parameters. The simple Equation 8 is considered a first-order approximation. Note also that Equation 8 is roughly consistent with the simulation results for a simple fracture network (Kwicklis and Healy 1993, pp. 4098-4099). Their results indicated that fracture flow generally occurs in a smaller number of fracture segments when the characteristic capillary pressure of the fracture network is reduced. Decreasing capillary pressure corresponds to decreasing fracture saturation.

6.4.5.2 Constitutive Relations

Note that only the active fracture continuum, a portion of the total fracture continuum, contributes to flow and transport in fractures and fracture-matrix interaction. Therefore, fracture hydraulic properties should be defined for active fractures. The effective water saturation of active fractures, S_{ae} (-), is related to the effective water saturation in connected fractures, S_e, by (Liu et al. 1998, p. 2636)

$$S_{ae} = \frac{S_e}{f_a} = S_e^{\,1-\gamma} \qquad \text{(Eq.10)}$$

Because $S_{ae} \leq 1$, γ should be less than or equal to one. The effective water saturation of active fractures is related to the actual water saturation in active fractures, S_a, by (Liu et al. 1998, p. 2636)

$$S_{ae} = \frac{S_a - S_r}{1 - S_r} \qquad \text{(Eq.11)}$$

If all connected fractures are considered to be active in conducting water, the water capillary pressure for the fracture continuum may be described by the well-known van Genuchten (V-G) relation (van Genuchten 1980, pp. 892-893):

$$P_c(S_e) = \frac{1}{\alpha}[S_e^{\,-1/m} - 1]^{1/n} \qquad \text{(Eq.12)}$$

where α, (Pa^{-1}), n, (-) and $m = 1\text{-}1/n$ are V-G parameters. In the active fracture model, however, the V-G capillary pressure relation is considered to be relevant for the active fracture continuum rather than for the whole fracture continuum. The capillary pressure for active fractures is determined by replacing S_e in Equation 11 with S_{ae},

$$P_c(S_e) = \frac{1}{\alpha}[S_{ae}^{\,-1/m} - 1]^{1/n} = \frac{1}{\alpha}[S_e^{\,(\gamma-1)/m} - 1]^{1/n} \qquad \text{(Eq.13)}$$

Equation 13 rather than 12 should be used to simulate water flow in the fracture continuum. Figure 3 shows fracture capillary pressure curves for several γ values. For a given effective water saturation in connected fractures, a larger γ value corresponds to a larger effective water saturation in active fractures and therefore to a lower absolute value for capillary pressure.

The liquid-phase relative permeability for the active fracture continuum, k_{ar} (-), is directly determined by the effective water saturation of active fractures. However, as only a portion of the fractures are active, the relative permeability of the entire fracture continuum, k_r (-), should be the relative permeability of active fractures multiplied by f_a, or (Liu et al. 1998, p. 2636).

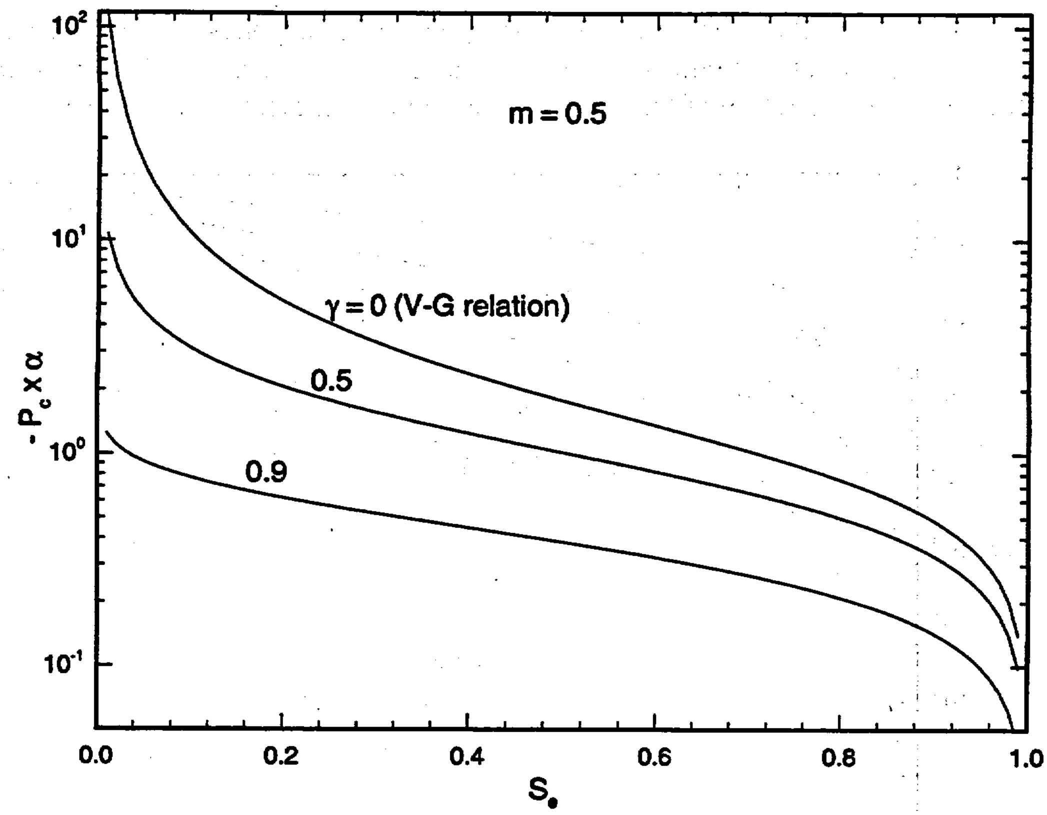

Figure 3. Capillary Pressure Curves of Fracture Continuum for γ = 0, 0.5 and 0.9 (Liu et al. 1998, p. 2636, Figure 2)

$$k_r = f_a k_{ar} = S_e^{\gamma} k_{ar} \qquad \text{(Eq.14)}$$

where k_{ar} can be given by the following V-G permeability relation (Liu et al. 1998, p. 2636):

$$k_{ar} = S_{ae}^{1/2}[1-\{1-S_{ae}^{1/m}\}^m]^2 = S_e^{(1-\gamma)/2}[1-\{1-S_e^{(1-\gamma)/m}\}^m]^2 \qquad \text{(Eq.15)}$$

Combining Equations 10 and 11 yields

$$k_r = S_e^{(1+\gamma)/2}[1-\{1-S_e^{(1-\gamma)/m}\}^m]^2 \qquad \text{(Eq.16)}$$

Relative permeability (k_r) curves are shown in Figure 4 for several γ values. In general, the relative permeability (k_r) is affected by γ in a complicated manner for a given S_e. A larger γ value, resulting in a higher effective water saturation in active fractures (S_{ae}), gives rise to a larger value of k_{ar}. On the other hand, a larger γ value corresponds to a smaller value of f_a. Because the former effect is dominant, a larger γ value gives a larger relative permeability for a given effective water saturation of the fracture continuum, as indicated in Figure 4.

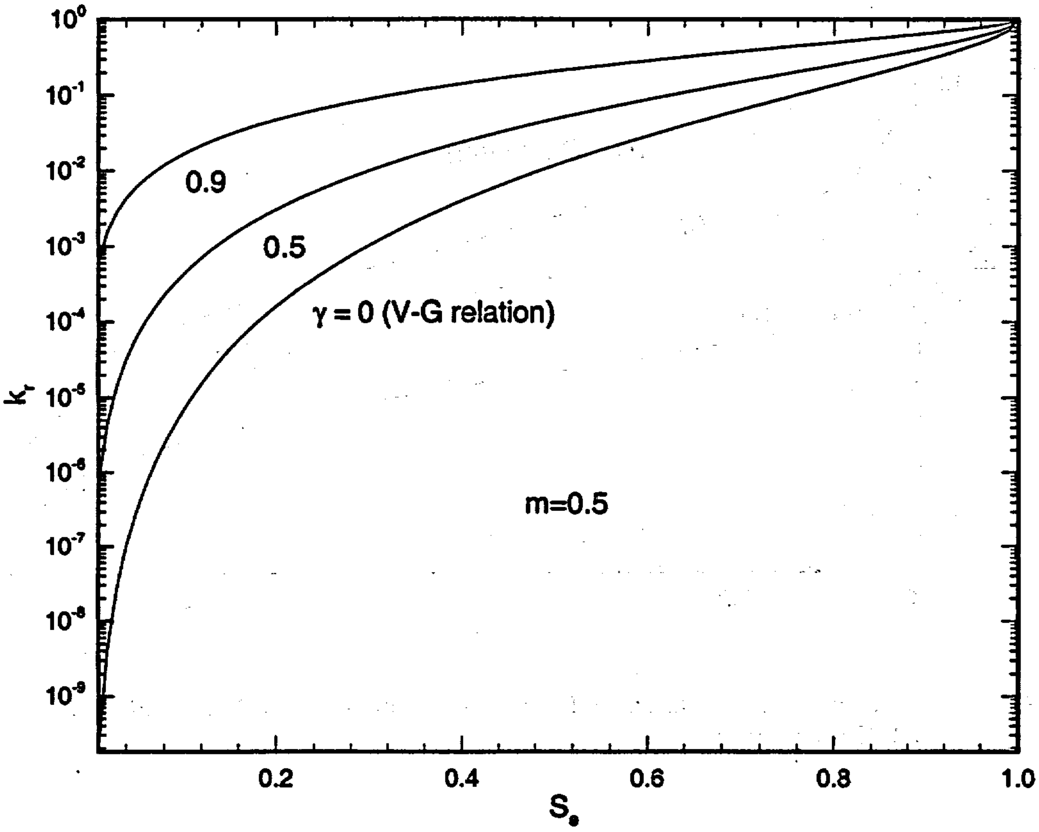

Figure 4. Relative Permeability Curves of Fracture Continuum for $\gamma = 0$, 0.5 and 0.9 (Liu et al. 1998, p. 2637, Figure 3)

In the active fracture model, the fracture-matrix interface-area reduction factor results from three aspects. First, the average interface area between mobile water (saturated liquid water segments) in an active fracture and the surrounding matrix is smaller than the geometric interface area. Second, the number of active fractures is smaller than that of connected fractures. Conventionally, all the connected fractures were considered to contribute to fracture-matrix interaction. Third, average active fracture spacing is much larger than that for connected fractures. Under the quasi-steady-state condition, flow and transport between fractures and surrounding matrix is inversely proportional to the corresponding fracture spacing. Based on these considerations and Equation 8, Liu et al. (1998, pp. 2636–2638) derived an approximate expression for the reduction factor:

$$R \cong S_e^{\,1+\gamma} \tag{Eq.17}$$

Note that the active fracture model uses a combination of the volume-averaged method and a simple filter to deal with fracture flow and transport. Inactive fractures are filtered out in modeling fracture-matrix interaction, flow, and transport in the fracture continuum. We believe that use of the filtering method could add a capability to continuum approaches for capturing dispersed fingering flow at a subgrid scale. A major limitation of continuum approaches was considered to be their inability to represent subgrid-scale fingering flow (Glass et al. 1996, p. 7). Note that the γ factor may be interpreted as a measure of the "activity" of connected fractures. Generally speaking, a smaller γ value corresponds to a larger number of active fractures in a connected fracture network. For example, $\gamma = 0$ results in $f_a = 1$ in Equation 8, corresponding to all connected fractures being active. On the other hand, $\gamma = 1$ corresponds to zero fracture capillary pressure (Equation 13), indicating that all active fractures are saturated. In the latter case, the fraction of active fractures is very small for small percolation fluxes because relatively high fracture permeabilities measured at Yucca Mountain allow most of the water to flow through only a few fractures. Note that the γ value cannot be determined by laboratory measurements of fractured core samples, because γ represents an inherently large-scale process. Instead, it must be inferred through inverse modeling using the site-scale UZ model and field-scale data collected at Yucca Mountain (Liu et al. 1999, p. 2638).

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7. CONCLUSIONS

A variety of flow and transport processes are involved in the UZ at Yucca Mountain. The conceptual model and numerical modeling approaches used for modeling these processes are summarized in this report.

Flow processes are considered to be characterized by the following attributes. Because of the expected attenuation effects of the PTn unit, the percolation processes below this unit are considered to be approximately in steady state under ambient conditions. Fracture liquid-water flow is dominant in a welded unit and matrix flow in a nonwelded unit. Many, dispersed fractures are actively conducting liquid water in the UZ of Yucca Mountain. Isolated, transient, and fast flow paths exist, but carry only a small amount of liquid water. Fracture-matrix interaction in the welded units is limited. The existence of the perched water bodies introduces three-dimensional lateral flow within the UZ.

Solute transport within the UZ of Yucca Mountain is closely tied to the conceptual model of flow. Advective transport pathways coincide with flow pathways. Matrix diffusion is a major mechanism for mass transfer between fractures and the matrix, and contributes to the retardation of radionuclide transport when fracture flow is dominant. Sorption can also act to retard the movement of radionuclides in the UZ: radionuclides and reactive chemicals, which are strongly sorbed to rock matrix, are relatively immobile. On the other hand, sorptive interactions may enhance radionuclide transport if the aqueous species sorbs to colloids. Dispersion is not expected to be a major transport mechanism in the UZ. In addition, perched water bodies may act as a mechanism to dilute solute and radionuclide plumes.

Flow and transport will be affected by coupled TH, TM and TC processes resulting from potential repository heat release. In general, the influence of radioactive decay heat includes: (1) vaporization of *in situ* liquid water, (2) thermally driven water vapor movement away from the heat sources, (3) condensation of water vapor in cooler regions, and (4) condensate reflux driven by gravity and capillary forces. Thermally induced mineralogical and mechanical property changes in the UZ also can alter the permeability and porosity, and therefore have further effects on flow and transport.

Several basic numerical approaches are available for modeling flow and transport in unsaturated, fractured rock. Based on flow and transport behavior in the UZ of Yucca Mountain, the scale of the problem, data availability, and computational feasibility, the dual-permeability approach is considered the most appropriate approach for modeling flow and transport processes. Relevant issues, such as the comparison between conventional approaches and particle-tracking methods for modeling transport processes, are addressed. The active fracture model, used to describe fracture-matrix interaction, is documented in this AMR.

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8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

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9. ATTACHMENTS

Attachment I – Document Input Reference Sheet

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ATTACHMENT I—DOCUMENT INPUT REFERENCE SHEET

DIRS as of the issue date of this AMR. Refer to the DIRS database for the current status of these inputs.

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DOCUMENT INPUT REFERENCE SHEET

JZH 4/17/00

1. Document Identifier No./Rev.: MDL-NBS-HS-000005/Rev. 00	Change: N/A	Title: Conceptual and Numerical Model for Unsaturated Zone Flow and Transport

Input Document							8. TBV Due To		
2a	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section	4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	Unqual.	From Uncontrolled Source	Un-confirmed
1.	Abdel-Salam, A. and Chrysikopoulos, C.V. 1996. "Unsaturated Flow in a Quisi-Three-Dimensional Fractured Medium with Spatially Variable Aperture." *Water Resources Research 32* (6), 1531–1540. Washington, D.C.: American Geophysical Union. TIC: 239861.	pp. 1537–1538	N/A-Reference only	6.1.3	Fracture-Matrix interaction	N/A	N/A	N/A	N/A
2.	Ahlers, C.F.; Finsterle, S.; and Bodvarsson, G.S. 1999. "Characterization and Prediction of Subsurface Pneumatic Response at Yucca Mountain, Nevada." *Journal of Contaminant Hydrology 38* (1–3), 47–68. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	p. 49 47, 58, 59–66	N/A-Reference only	6.1.2 6.1.8	Pneumatic response	N/A	N/A	N/A	N/A
3.	Bear, J.; Tsang, C.F.; and de Marsily, G. eds., 1993. *Flow and Contaminant Transport in Fractured Rock.* San Diego, California: Academic Press. TIC: 226388.	pp. 267–320, 396–428 395–396, 3–10 419	N/A-Reference only	6.4.1 6.4.1.1.1 6.4.4	Numerical modeling of fracture flow and transport	N/A	N/A	N/A	N/A

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2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
2a									
4.	Bandurraga, T.M. and Bodvarsson, G.S. 1999. "Calibrating Hydrogeologic Parameters for the 3-D Site-Scale Unsaturated Zone Model of Yucca Mountain, Nevada." *Journal Of Contaminant Hydrology 38* (1–3), 25–46. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	p. 40, table 3	N/A-Reference only	6.1.2	Liquid travel times in fractures and matrix	N/A	N/A	N/A	N/A
5.	Bodvarsson, G.S.; Boyle, W.; Patterson, R.; and Williams, D. 1999. "Overview of Scientific Investigations at Yucca Mountain—the Potential Repository for High-Level Nuclear Waste." *Journal of Contaminant Hydrology 38* (1–3), 3–24. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	pp. 8–10, 10 11 13 14–15 13	N/A-Reference only	6 6.1.1, 6.1.2 5, 6.1.2 6.1.3 6.1.4 6.1.7	Flow processes in the UZ	N/A	N/A	N/A	N/A

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2. Technical Product Input Source Title and Identifier(s) with Version		3. Section	4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	Unqual.	From Uncontrolled Source	Un-confirmed
2a									
6.	Brooks, R.H. and Corey, A.T. 1966. "Properties of Porous Media Affecting Fluid Flow." *Journal of Irrigation and Drainage Division: Proceedings of the American Society of Civil Engineers, 92* (IR2), 61–88. Washington, D.C.: American Society of Civil Engineers. TIC: 216867.	p. 71	N/A-Reference only	6.4.4	Relative permeability of gas flow	N/A	N/A	N/A	N/A
7.	Buscheck, T.A. and Nitao, J.J. 1993. "Repository-Heat-Driven Hydrothermal Flow at Yucca Mountain, Part I: Modeling and Analysis." *Nuclear Technology, 104* (3), 418–448. La Grange Park, Illinois: American Nuclear Society. TIC: 224039.	pp. 418–448	N/A-Reference only	6.3.1	pH processes	N/A	N/A	N/A	N/A
8.	Clemo, T. and Smith L. 1997. "A Hierarchical Model for Solute Transport in Fractured Media" *Water Resources Research 33* (8), 1763–1783. Washington, D.C.: American Geophysical Union. TIC: 239864.	pp. 1763–1765	N/A-Reference only	6.4.2	Models for flow and transport in fractures	N/A	N/A	N/A	N/A

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2. Technical Product Input Source Title and Identifier(s) with Version		3. Section	4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	Unqual.	From Uncontrolled Source	Un-confirmed
2a									
9.	Conca, J.L. and Wright, J. 1990. "Diffusion Coefficients in Gravel Under Unsaturated Conditions." *Water Resources Research 26* (5), 1055–1066. Washington, D.C.: American Geophysical Union. TIC: 237421.	p. 1055	N/A-Reference only	6.2.2	Relation between the diffusion coefficient and water content	N/A	N/A	N/A	N/A
10.	CRWMS M&O 1998. *Unsaturated Zone Radionuclide Transport*. Chapter 7 of *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document*. B00000000-01717-4301-00007-01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0007.	section 7.2.3	N/A-Reference only	6.2.5	Dispersion	N/A	N/A	N/A	N/A
11.	CRWMS M&O (Civilian Radioactive Waste Management System, Management & Operating Contractor) 1999a. *M&O Site Investigations*. Activity Evaluation. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990317.0330.	Entire	N/A - Reference only	2	Activity Evaluation	N/A	N/A	N/A	N/A

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2. Technical Product Input Source Title and Identifier(s) with Version		3. Section	4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	Unqual.	From Uncontrolled Source	Un-confirmed
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12.	CRWMS M&O 1999b. *M&O Site Investigations.* Activity Evaluation. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990928.0224.	Entire	N/A - Reference only	2	Activity Evaluation	N/A	N/A	N/A	N/A
13.	CRWMS M&O 1999c. *Analysis & Modeling Development Plan (DP) for U0030 Conceptual and Numerical Model for Unsaturated Zone Flow and Transport Rev. 00.* TDP-NBS-HS-0000010. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990830.0379.	Entire	N/A - Reference only	2	Development Plan for this AMR	N/A	N/A	N/A	N/A
14.	de Marsily, G. 1986. *Quantitative Hydrogeology and Groundwater Hydrology for Engineers.* Orlando, Florida: Academic Press. TIC: 226335.	pp. 270–272 265, 234–235, 244, 236–238	N/A-Reference only	6.2.4 6.2.5	Transport processes	N/A	N/A	N/A	N/A

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2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
2a									
15.	DOE (U.S. Department of Energy) 1998. "Total System Performance Assessment." Volume 3 of *Viability Assessment of a Repository at Yucca Mountain.* DOE/RW-0508. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19981007.0030.	3-165–3-166 3-118 3-105	N/A-Reference only	6.1.6 6.2.3 6.2.4	Transient flow Sorption Colloid-facilitated transport	N/A	N/A	N/A	N/A
16.	Domenico, P.A. and Schwartz, F.W. 1990. *Physical and Chemical Hydrogeology.* New York, New York: John Wiley and Sons. TIC: 234782.	440–443	N/A-Reference only	6.2.3	K_d approach Sorption	N/A	N/A	N/A	N/A
17.	Doughty, C. 1999. "Investigation of Conceptual and Numerical Approaches for Evaluating Moisture, Gas, Chemical, and Heat Transport in Fractured Unsaturated Rock." *Journal of Contaminant Hydrology 38* (1–3), 69–106. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	p. 76 77 94–95, 80–82	N/A-Reference only	6.4.1.1.3 6.4.2 6.4.4	Modeling of flow and transport in fractured media	N/A	N/A	N/A	N/A

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Input Document							8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section	4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	Unqual.	From Uncontrolled Source	Un-confirmed
2a									
18.	Dyer, J.R. 1999. "Revised Interim Guidance Pending Issuance of New U.S. Nuclear Regulatory Commission (NRC) Regulations (Revision 01, July 22, 1999), for Yucca Mountain, Nevada." Letter from J.R. Dyer (DOE) to D.R. Wilkins (CRWMS M&O), September 9, 1999, OL&RC:SB-1714, with enclosure, "Interim Guidance Pending Issuance of New U.S. Nuclear Regulatory Commission (NRC) Regulations (Revision 01)." ACC: MOL.19990910.0079.	Entire	N/A Reference only	4.2	Interim Guidance	N/A	N/A	N/A	N/A

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Input Document							8. TBV Due To		
2a	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section	4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	Unqual.	From Uncontrolled Source	Un-confirmed
19.	Fabryka-Martin, J. T.; Wolfsberg, A. V.; Roach, J.L.; Levy, S. S.; Winters, S. T.; Wolfsberg, L.E.; Elmore, D.; and Sharma, P. 1998. "Distribution of Fast Hydrologic Paths in the Unsaturated Zone at Yucca Mountain." *Proceedings of the Eighth International Conference on High-Level Radioactive Waste Management, Las Vegas, Nevada, May 11–14, 1998,* 93–96. La Grange Park, Illinois: American Nuclear Society. TIC: 237957.	p. 93 pp. 93–94 p. 96	N/A-Reference only	6.1.2 6.1.3, 6.1.5 6.1.7	Flow paths in the UZ	N/A	N/A	N/A	N/A
20.	Fetter, C.W. 1993. *Contaminant Hydrogeology.* New York, New York: Macmillan Publishing. TIC: 240691.	P 47 117, 149–150 149	N/A-Reference only	6.2.1 6.2.3 6.2.4	Transport processes	N/A	N/A	N/A	N/A

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2a									
21.	Flint, L.E.; Flint, A.L.; and Hevesi, J.A. 1994. "Shallow Infiltration Processes in Arid Watersheds at Yucca Mountain, Nevada." *Proceedings of the Fifth Annual International Conference on High Level Radioactive Waste Management, Las Vegas, Nevada, 4, May 22–26, 1994,* 2315–2322. La Grange Park, Illinois: American Nuclear Society. TIC: 210984.	pp. 2315–2322	N/A-Reference only	6.1.1	Infiltration processes	N/A	N/A	N/A	N/A
22.	Flint, L.E. 1998. *Characterization of Hydrogeologic Units Using Matrix Properties, Yucca Mountain, Nevada.* Water-Resources Investigations Report 97-4243. Denver, Colorado: U.S. Geological Survey. TIC: 236515.	pp. 29–33 24–30 24–30	N/A-Reference only	6.1.2 6.1.7 6.4.3	Hydrologic property; matrix saturation distribution	N/A	N/A	N/A	N/A
23.	Freeze, R.A. and Cherry, J.A. 1979. *Groundwater.* Englewood Cliffs, New Jersey: Prentice-Hall. TIC: 3476.	p. 45	N/A-Reference only	6.1.4	Perched water	N/A	N/A	N/A	N/A

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2a									
24.	Glass, R.J.; Nicholl, M.J.; and Tidwell, V.C. 1996. *Challenging and Improving Conceptual Models for Isothermal Flow in Unsaturated, Fractured Rock through Exploration of Small-Scale Processes.* SAND95-1824. Albuquerque, New Mexico: Sandia National Laboratories. ACC: MOL.19960620.0014.	pp. 6–7 7	N/A-Reference only	6.1.3 6.4.5.2	Fingering flow in fractures	N/A	N/A	N/A	N/A
25.	Hardin, E.L. 1998. *Near-Field/Altered Zone Models Report.* Milestone SP3100M4. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980630.0560.	pp. 2-2, 2-3, 2-8	N/A-Reference only	6.3.3	Coupled processes	N/A	N/A	N/A	N/A
26.	Haukwa, C. B.; Wu, Y.S.; and Bodvarsson, G.S. 1999. "Thermal Loading Studies Using the Yucca Mountain Unsaturated Zone Model." *Journal of Contaminant Hydrology 38* (1–3), 217–255. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	pp. 227, 247–248	N/A-Reference only	6.3.1	T-H processes	N/A	N/A	N/A	N/A

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							Unqual.	From Uncontrolled Source	Un-confirmed
2a									
27.	Hevesi, J.A.; Ambos, D.S.; and Flint, A.L. 1994. "A Preliminary Characterization of the Spatial Variability of Precipitation at Yucca Mountain, Nevada." *Proceedings of the Fifth Annual International Conference on High Level Radioactive Waste Management, Las Vegas, Nevada, 4, May 22-26,1994,* 2520-2529. La Grange Park, Illinois: American Nuclear Society. TIC: 222058.	Entire	N/A-Reference only	6.1.1	Infiltration processes	N/A	N/A	N/A	N/A

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2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
2a									
28.	Ho, C.K. 1997. "Models of Fracture-Matrix Interactions during Multiphase Heat and Mass Flow in Unsaturated Fractured Porous Media." *The Sixth Symposium on Multiphase Transport in Porous Media, ASME International Mechanical Engineering Congress and Exposition, November 16-24, 1996, Dallas, Texas.* New York, New York: American Society of Mechanical Engineers. TIC: 234839.	pp. 401–412	N/A-Reference only	6.1.3	Fracture-matrix interaction	N/A	N/A	N/A	N/A
29.	Kneafsey, T.J. and Pruess. K. 1998. "Thermohydrological Laboratory Tests-Insights into Processes and Behavior." *Proceedings of the Eighth International Conference on High-Level Radioactive Waste Management, Las Vegas, Nevada, May 11–14, 1998,* 261–263. La Grange Park, Illinois: American Nuclear Society. TIC: 237082.	p. 263	N/A-Reference only	6.3.1	T-H processes	N/A	N/A	N/A	N/A

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2a									
30.	Kwicklis, E.M. and Healey, R.W. 1993. "Numerical Investigation of Steady Liquid Water Flow in a Variably Saturated Fracture Network." *Water Resources Research 29* (12), 4091–4102. Washington, D.C.: American Geophysical Union. TIC: 226993.	pp. 4097–4099 4091–4102 4097–4099	N/A-Reference only	6.1.3 6.4.1.2 6.4.5.1	Flow in fracture networks	N/A	N/A	N/A	N/A
31.	LeCain, G.D. 1997. *Air-Injection Testing in Vertical Boreholes in Welded and Nonwelded Tuff, Yucca Mountain, Nevada.* Water Resources Investigations Report 96-4262. Denver, Colorado: U.S. Geological Survey. ACC: MOL.19980310.0148.	pp. 31–32	N/A-Reference only	6.4.4	Fracture permeability	N/A	N/A	N/A	N/A
32.	Leverett, M.C. 1941. "Capillary Behavior in Porous Solids." *AIME Transactions, 142.* New York, New York: American Institute of Mining, Metallurgical and Petroleum Engineers. TIC: 240680.	157–169	N/A-Reference only	6.3.2	TM formulation for capillary pressure	N/A	N/A	N/A	N/A

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2a									
33.	Liu, H.H.; Doughty, C.; and Bodvarsson, G.S. 1998. "An Active Fracture Model for Unsaturated Flow and Transport in Fractured Rocks." *Water Resources Research 34* (10), 2633–2646. Washington, D.C.: American Geophysical Union. TIC: 243012.	2633–2645 2635 2635–2636 2636–2638	N/A-Reference only	6.1.3 6.1.7 6.4.5.1 6.4.5.2	Active fracture model	N/A	N/A	N/A	N/A
34.	Millington, R.J. and Qirk, J.M. 1961. "Permeability of Porous Solids." *Journal of the Chemical Society, Faraday Transactions, 57,* 1200–1207. Toronto, Canada: Royal Society of Chemistry. TIC: 246707	Entire	N/A-Reference only	6.2.2	Matrix diffusion	N/A	N/A	N/A	N/A
35.	Montazer, P. and Wilson, W.E. 1984. *Conceptual Hydrologic Model of Flow in the Unsaturated Zone, Yucca Mountain, Nevada.* Water-Resources Investigations Report 84-4345. Denver, Colorado: U.S. Geological Survey. TIC: 203223.	9–20, 36–49 45–47 20 36–51 51	N/A-Reference only	6 5, 6.1.2 6.1.5 6.1.9 6.2.5	Conceptual model of flow	N/A	N/A	N/A	N/A

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2a									
36.	National Research Council. 1996. *Rock Fractures and Fluid Flow, Contemporary Understanding and Applications.* Washington, D.C.: National Academy Press. TIC: 235913.	307–394 332–350 331 380	N/A-Reference only	6.4.1 6.4.1.2 6.4.2 6.4.4	Approaches for modeling flow and transport in fractured porous media	N/A	N/A	N/A	N/A
37.	Neretnieks, I. 1993. "Solute Transport in Fractured Rock—Applications to Radionuclide Waste Repositories." *Flow and Contaminant Transport in Fractured Rock*, 39–127. Bear, J.; Tsang, C.F.; and de Marsilly, G. eds. San Diego, California: Academic Press. TIC: 235461.	47–48	N/A-Reference only	6.2.2	Matrix diffusion	N/A	N/A	N/A	N/A
38.	Nitao, J.J. and Buscheck, T.A. 1991. "Infiltration of a Liquid Front in an Unsaturated Fractured Porous Media." *Water Resources Research, 27* (8), 2099-2112. Washington, D.C.: American Geophysical Union. TIC: 224848.	Entire	N/A-Reference only	6.1.9 6.2.5	Conceptual model	N/A	N/A	N/A	N/A

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2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
2a									
39.	Paces, J.B.; Neymark, L.A.; Marshall, B.D.; Whelan, J.F.; and Peterman, Z.E. 1998. "Inferences for Yucca Mountain Unsaturated-Zone Hydrology From Secondary Minerals." *Proceedings of the Eighth International Conference on High-Level Radioactive Waste Management, Las Vegas, Nevada, May 11–14, 1998,* 36–39. La Grange Park, Illinois: American Nuclear Society. TIC: 238482.	p. 37	N/A-Reference only	6.1.2	Implication of calcite coating	N/A	N/A	N/A	N/A
40.	Peters, R.R. and Klavetter, E.A. 1988. "Continuum Model for Water Movement in an Unsaturated Fractured Rock Mass." *Water Resources Research, 24* (3), 416–430. Washington, D.C.: American Geophysical Union. TIC: 212757.	416–430	N/A-Reference only	6.1.9 6.2.5	Conceptual Model	N/A	N/A	N/A	N/A

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2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
2a									
41.	Pruess, K. 1999. "A Mechanistic Model for Water Seepage through Thick Unsaturated Zones in Fractured Rocks of Low Permeability." *Water Resources Research, 35* (4), 1039-1051. Washington, D.C.: American Geophysical Union. TIC: 244913.	1039–1051	N/A-Reference only	6.1.9 6.2.5	Conceptual model	N/A	N/A	N/A	N/A
42.	Pruess, K. and Narasimhan, T.N. 1985. "A Practical Method for Modeling Fluid and Heat Flow in Fractured Porous Media." *Society of Petroleum Engineers Journal, 25* (1), 14-26. Dallas, Texas: Society of Petroleum Engineers. TIC: 221917.	pp. 14–26	N/A-Reference only	6.4.1.1.4	MINC approach	N/A	N/A	N/A	N/A
43.	Pruess, K. and Tsang, Y.W. 1994. *Thermal Modeling for a Potential High-Level Nuclear Waste Repository at Yucca Mountain, Nevada.* Report LBL-35381, UC-600. Berkeley, California: Lawrence Berkeley National Laboratory. ACC: NNA.19940427.0248.	pp. 47–49	N/A-Reference only	6.4.1.1.2	The EMC approach	N/A	N/A	N/A	N/A

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2a									
44.	Pruess, K.; Faybishenko, B. and Bodvarsson, G.S. 1999. "Alternative Concepts and Approaches for Modeling Flow and Transport in Thick Unsaturated Zones of Fractured Rocks." *Journal of Contaminant Hydrology 38* (1–3), 281–322. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	p. 283 308	N/A-Reference only	6.1.2 6.4.1.2, 6.4.2	The conceptual model of lfow and transport	N/A	N/A	N/A	N/A
45.	Ritcey, A.C. and Wu, Y.S. 1999. "Evaluation of the Effect of Future Climate Change on the Distribution and Movement of Moisture in the Unsaturated Zone at Yucca Mountain, NV." *Journal of Contaminant Hydrology* 38 (1–3), 257–279. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	pp. 262–268	N/A-Reference only	5, 6.1.2	Lateral flow within PTn	N/A	N/A	N/A	N/A

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2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
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46.	Robinson, B.A.; Wolfsberg, A.V.; Gable, C.W.; and Viswanathan, H.S. 1998. "Radionuclide Transport in the Unsaturated Zone at Yucca Mountain." *Proceedings of the Eighth International Conference on High-Level Radioactive Waste Management, Las Vegas, Nevada, May 11–14, 1998, 156–158.* La Grange Park, Illinois: American Nuclear Society. TIC: 237082.	157	N/A-Reference only	6.3.1	UZ transport	N/A	N/A	N/A	N/A
47.	Rousseau, J.P.; Kwicklis, E.M.; and Gillies, D.C., eds. 1999. *Hydrogeology of the Unsaturated Zone, North Ramp Area of the Exploratory Studies Facility, Yucca Mountain, Nevada.* Water-Resources Investigations Report 98-4050. Denver, Colorado: U.S. Geological Survey. TIC: 243099.	89 143–161 89–97 77–110	N/A-Reference only	6.1.2 6.1.7 6.1.8 6.4.4	Gas flow in Tcw; Water potential measurements; pneumatic pressure Gas flow in welded units. Temperature measurements	N/A	N/A	N/A	N/A

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2a									
48.	Sharp J.M.; Kreisel, J.I.; and Milliken K.L. 1996. "Fracture Skin Properties and Effects on Solute Transport: Geotechnical and Environmental Implications." *Rock Mechanics*. Balkema, Rotterdam. TIC: 239941.	p. 1331	N/A-Reference only	6.1.3	Effects of fracture coatings on flow and transport	N/A	N/A	N/A	N/A
49.	Sonnenthal, E. L. and Bodvarsson, G. S. 1999. "Constraints on the Hydrology of the Unsaturated Zone at Yucca Mountain, NV from Three-Dimensional Models of Chloride and Strontium Geochemistry." *Journal of Contaminant Hydrology 38* (1–3), 107–156. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	pp. 118, 151	N/A-Reference only	6.2.5	Perched water	N/A	N/A	N/A	N/A

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2a									
50.	Thoma, S.G.; Gallegos, D.P.; and Smith, D.M. 1992. "Impact of Fracture Coatings on Fracture-Matrix Flow Interactions in Unsaturated, Porous Media." *Water Resources Research 28* (5), 1357–1367. Washington, D.C.: American Geophysical Union. TIC: 237509.	pp. 1357–1367	N/A-Reference only	6.1.3	Effects of fracture coating on flow and transport	N/A	N/A	N/A	N/A
51.	Thorstenson, D.C.; Weeks, E.P.; Haas, H.; and Woodward, J.C. 1989. "Physical and Chemical Characteristics of Topographically Affected Airflow in an Open Borehole at Yucca Mountain, Nevada." *Proceedings of the Topical Meeting on Nuclear Waste Isolation in the Unsaturated Zone FOCUS '89, Las Vegas, Nevada, September 17–21, 1989*, 256–270. Las Vegas, Nevada: American Nuclear Society. TIC: 216833.	p. 262	N/A-Reference only	6.1.8	Gas flow processes	N/A	N/A	N/A	N/A

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2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
2a									
52.	Tokunaga, T.K. and Wan, J. 1997. "Water Film Flow along Fracture Surfaces of Porous Rock." *Water Resources Research 33* (6), 1287–1295. Washington, DC: American Geophysical Union. TIC: 242739.	pp. 1287–1295	N/A-Reference only	6.1.3	Film flow in fractures	N/A	N/A	N/A	N/A
53.	Triay, I.R.; Meijer, A.; Conca, J.L.; Kung, K.S.; Rundberg, R.S.; Strietelmeier, B.A.; and Tait, C.D. 1997. *Summary and Synthesis Report on Radionuclide Retardation for the Yucca Mountain Site Characterization Project.* Milestone Report MS-3784M. Los Alamos, New Mexico: Los Alamos National Laboratory. ACC: MOL.19971210.0177.	p. 173	N/A-Reference only	6.2.3	Transport processes	N/A	N/A	N/A	N/A

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2a									
54.	Tsang, Y.W. and Birkholzer, J.T. 1999. "Predictions and Observations of the Thermal-Hydrological Conditions in the Single Heater Test." *Journal of Contaminant Hydrology 38* (1–3), 385–425. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	389–390	N/A-Reference only	6.3.1	TH processes	N/A	N/A	N/A	N/A
55.	van Genuchten, M. 1980. "A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils." *Soil Science Society of America Journal, 44* (5), 892–898. Madison, Wisconsin: Soil Science Society of America. TIC: 217327.	892–893 892–898 892–893	N/A-Reference only	5 6.4.4 6.4.5.2	van Genuchten relations	N/A	N/A	N/A	N/A

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56.	Wang J.S.Y. and Narasimhan T.N. 1993. "Unsaturated Flow in Fractured Porous Media." Chapter 7 of *Flow and Contaminant Transport in Fractured Rocks.* Bear, J.; Tsang, C.F.; and de Marsily, G., eds. New York, New York: Academic Press. TIC: 235461.	354–361 354–361 329–335 354–361 374–377 327–339 327–339	N/A-Reference only	5 6.1.2 6.1.3 6.1.6 6.1.7 6.1.9 6.2.5	Flow and transport in the UZ	N/A	N/A	N/A	N/A
57.	Wang, H.F.; Blair, S.C.; and Berge, P.A. 1998. "Estimating Changes in Rock Permeability Due to Thermal-Mechanical Effects." *Proceedings of the Eighth International Conference on High-Level Radioactive Waste Management, Las Vegas, Nevada, May 11–14, 1998,* 108–110. La Grange Park, Illinois: American Nuclear Society. TIC: 237082.	pp. 108–110	N/A-Reference only	6.3.2	TM processes	N/A	N/A	N/A	N/A

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2a									
58.	Warren, J.E. and Root, P.J. 1963. "The Behavior of Naturally Fractured Reservoirs." *Society of Petroleum Engineers Journal, 228,* 245–255. Dallas, Texas: Society of Petroleum Engineers. TIC: 233671.	pp. 245–255	N/A-Reference only	6.4.1.1.3	Continuum approach	N/A	N/A	N/A	N/A
59.	Weeks, E.P. 1987. "Effect of Topography on Gas Flow in Unsaturated Fractured Rock: Concepts and Observations." *Flow And Transport Through Unsaturated Fractured Rock,* 165–170. Evans, D.D. and Nicholson, T.J., eds. Geophysical Monograph 42. Washington, D.C.: American Geophysical Union. TIC: 223605..	pp. 165–170	N/A-Reference only	6.1.8	Gas flow processes	N/A	N/A	N/A	N/A

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2a									
60.	Wemheuer, R.F. 1999. "First Issue of FY00 NEPO QAP-2-0 Activity Evaluations." Interoffice correspondence from R.F. Wemheuer (CRWMS M&O) to R.A. Morgan (CRWMS M&O), October 1, 1999, LV.NEPO.RTPS.TAG.10/99-155, with attachments, Activity Evaluation for Work Package #1401213UM1. ACC: MOL.19991028.0162.	Work Package #1401213UM1	N/A-Reference only	4.2	Activity Evaluation	N/A	N/A	N/A	N/A
61.	Wu, Y.S.; Ritcey, A.C. and Bodvarsson, G.S. 1999a. "A Modeling Study of Perched Water Phenomena in the Unsaturated Zone at Yucca Mountain." *Journal Of Contaminant Hydrology 38* (1–3), 157–184. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	159–163 158–163	N/A-Reference only	6.1.2 6.1.4	Perched water	N/A	N/A	N/A	N/A

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1. Document Identifier No./Rev.:	Change:	Title:
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Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
2a									
62.	Wu, Y.S.; Haukwa, C. and Bodvarsson, G.S. 1999b. "A Site-Scale Model for Fluid and Heat Flow in the Unsaturated Zone of Yucca Mountain, Nevada." *Journal of Contaminant Hydrology 38* (1–3), 185–215. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	pp. 194–195	N/A-Reference only	6.4.1.1.2	Numerical approach	N/A	N/A	N/A	N/A
63.	Yang, I.C.; Rattray, G.W.; and Yu, P. 1996. *Interpretation of Chemical and Isotopic Data from Boreholes in the Unsaturated Zone at Yucca Mountain.* Water-Resources Investigations Report 96-4058. Denver, Colorado: U.S. Geological Survey. ACC: MOL.19970715.0408.	p. 34 55 34	N/A-Reference only	6.1.2 6.1.3 6.1.4	Perched water ^{14}C ages	N/A	N/A	N/A	N/A

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AP-3.15Q.1

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