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The influence of coatings and fills on flow in fractured, unsaturated tuff porous media systems

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Abstract. A numerical study of a single fracture embedded in a porous matrix was performed to investigate the role of fracture coatings and fills on water movement in permeable, fractured porous media. The variables considered were conductivity and continuity of fracture coatings; location, length, and conductivity of fracture fills; combinations of fills and coatings; initial matrix saturation; and inflow boundary conditions. Results from the simulations indicate that in low-saturation, high-capillarity tuff systems, the conditions under which fractures act as rapid flow paths are limited. These conditions include a continuous coating with conductivity several orders of magnitude lower than that of the neighboring matrix, and large inflow rates. However, as initial matrix saturation increases, the amount of fracture flow also increases. Discontinuities in coatings substantially reduce their effectiveness in preventing matrix imbibition. The presence of any coating, however, does produce increased infiltration depths. Fills appear to be effective barriers to fracture flow.

1. Introduction/Background

There is strong interest in fracture flow from a number of different arenas, including groundwater management and waste disposal. Arid environments, such as Yucca Mountain, Nevada, (YMP), Hanford, Washington, and Los Alamos National Laboratory, New Mexico (LANL), are being considered or have been used as waste disposal sites for radioactive and mixed wastes because of the presumed benefits of low infiltration rates; however, these sites are often in or near highly fractured media. The role that fractures play in these unsaturated systems is a challenging topic of study because of the myriad of complexities and interacting physical processes. There is concern about the potential for fractures to be major or fast paths for transporting water from the surface, or from disposal areas, through the subsurface and into groundwater supplies.

Under what conditions fractures may act as fast flow paths remains in question. Although the presence of coatings and fills in fractures has been documented, little is known about how they affect fluid flow and chemical transport. In the work presented here, we attempt to increase our understanding of the role of coatings and fills through computational modeling. We utilize a single fracture system with coatings and fills to investigate how different observed characteristics of fractures affect flow behavior and matrix-fracture interaction. Although the material parameters we used were from two different fractured, tuffaceous materials, the intention was not simply to answer a specific question for a specific location. We have, perhaps, taken some liberties with parameters to attempt to capture a more generic response. We hope that the information obtained from these studies can be extrapolated, to some extent, to an understanding of the behavior of the complete, more complex system.

In this work we are specifically concerned with unsaturated, fractured porous media within permeable matrix rocks. Although there have been hundreds of field and modeling efforts directed towards better understanding and representation of flow and transport in fractured porous media systems, only a fraction of these concern unsaturated, permeable materials. The role of fractures in unsaturated systems differs significantly from their role in saturated systems, with the existence of a permeable media often strongly affecting flow behavior [*Evans and Nicholson*, 1987]. Thus saturated and impermeable matrix studies offer only minor insight into the issues investigated here.

There have been observations on cores indicating the presence of fills and coatings [*Davidson and Snowdon*, 1978; *Carlos*, 1985] and analyses of the geophysical properties of fracture coating materials on tuffs [*Davenport*, 1995; *Carlos*, 1985]. On Yucca Mountain tuff samples from the vadose zone, observed fracture coatings are extremely discontinuous and sporadic [*Carlos et al.*, 1985]. *Carlos* [1985] reports coatings on the Topopah Spring tuff to be composed of a variety of minerals, including zeolites, mordenite, heulandite, and various clays. At Los Alamos, *Davenport et al.* [1995] report that the Bandelier Tuff coatings are predominantly clays (smectites) and calcites. Although fracture coating mineralogy has been determined, thickness and continuity have not been identified.

There have been a few published studies which have, either experimentally or numerically, tested the influence of a fracture coating, or "skin," on fracture-matrix interactions. *Thoma et al.* [1992] and *Chekuri et al.* [1995] ran experiments on actual coated and uncoated tuff fractures and did simple analytical or numerical analysis of the competition between capillary forces and viscous forces between the matrix and fracture. *Thoma et al.* [1992] observed that the lower permeability coatings inhibited matrix uptake and thus increased the depth that a water slug could potentially travel in a fracture. Their experiments also showed that a very low permeability coating (10^{-7} lower than the matrix) effectively eliminated matrix imbibition. Their simple one-dimensional analytical model was in good agreement with the observed matrix uptake. *Chekuri et al.* [1995]

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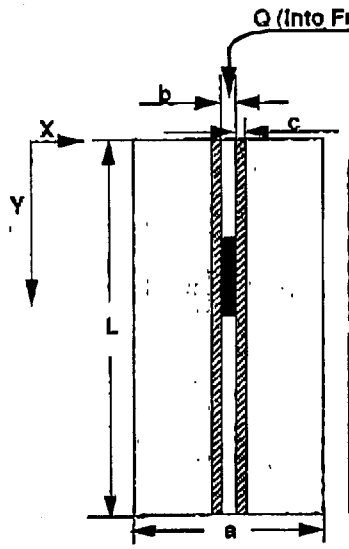


Dimension	Var.	Tuff A (meters)	Tuff B
System Length	L	2.5	15
Fracture Spacing	a	0.2	2.0
Fracture Aperture	b	1.2e-4	5e-3
Coating Thickness	c	3e-5	2e-4

Symbol	Material	Ksat (m/s)	Porosity	α(1/m)	N
	Matrix Tuff A	1.7e-11	0.10	0.005	1.8
	Matrix Tuff B	1.3e-06	0.46	0.3	1.9
	Fracture	7.2e-03	0.9	18.4	4.2
	Coating Fill (Tuff B)	9.5e-09 9.5e-11	0.2	0.152	1.17

Figure 1. System configuration for the matrix block/single fracture. Tables give dimensions and parameter values for the two simulated systems.

tested specimens from two Yucca Mountain tuffs: Tiva Canyon and Topopah Springs. Their experiments demonstrated mixed results, ranging from a slight increase to a measurable decrease in the effective permeability of a coated surface compared to a fresh surface. The results from Tiva Canyon showed little consistent influence of coatings, while the Topopah Springs samples showed a consistent decrease in water uptake by the matrix with coated fractures versus uncoated samples.

Nativ et al. [1995] conducted a field study in a near-saturated, fractured, low-permeability chalk in the Negev Desert. They observed rapid contaminant migration and concluded that at this site the fractures act as fast paths following precipitation events. The fracture fast paths result from the high background matrix saturation and low matrix permeability. In this study we will be focusing on systems with somewhat higher matrix permeability and generally lower saturations than the Negev chalk.

Pruess and Wang [1987] showed the result of a simple one-dimensional study of the effects of coating conductivity on matrix imbibition from a saturated fracture. They showed that the fracture coating caused a delay in the time required for the matrix to desaturate the fracture. *Ho* [1995] presented a modeling study that looked, in part, at the effects of reduced conductance between fracture and matrix in a dual permeability model. Ho achieved this by reducing the area of connection between the fracture and matrix by 2 orders of magnitude, as opposed to placing actual coating elements into the system. In that work Ho concluded that the reduced interaction had significant effect by reducing matrix saturations and increasing fracture velocity. *Moench* [1984] used the concept of a skin between the fracture and matrix to develop a double porosity model that was consistent for both transient and steady state assumptions regarding fracture-matrix interactions. The case study presented by Moench, based on his numerical derivation, showed at least minor effects, and sometimes large effects of a lower permeability layer between fracture and matrix.

Fractures have been suspected and identified as short circuit flow paths under conditions that are within the scope of those of concern in this study. Chlorine 36 measurements at Yucca Mountain have shown small quantities of bomb pulse ^{36}Cl at depths greater than 400 m. Modeling studies by *Wolfsberg et al.* [1996] have shown that this can be attributed to isolated rapid transport through fractures.

Continuing concerns about the role of fractures, along with these reported results demonstrate the importance of considering fracture wall coatings in predicting the influence of fractures. All of the previous studies assume a continuous coating, or "averaged" coating effect, and most apply only simple one-dimensional matrix imbibition. The current study specifically focuses on conditions that may strongly influence fracture flow and have not been considered previously. Although we have selected two "real" systems to apply this study, the greater purpose is to look at the sensitivities of certain classes of systems to potential fracture conditions. The work reported here expands the analysis of the influence of fractures by considering a wider range of conditions and by applying a more rigorous modeling approach. The presence of coatings as well as the possibility of fills is included. The influence of discontinuous coatings is also examined, and the response to discrete discontinuities is tested. The roles of initial matrix saturation and inflow conditions are also considered. We model a fully two-dimensional flow system using a multiphase finite element method (FEM) simulator. The modeling approach is described in section 2. Section 3 is a presentation of the observations from the simulations, while discussion and interpretation of those observations are left to section 4. Section 5 summarizes the work.

2. Method

The approach used in this work was to isolate and numerically study the role of specific aspects of a fracture-matrix system (e.g., coatings and fills) in conducting water in an unsaturated domain with permeable matrix materials. We chose a simple system containing a single vertical fracture centered in an otherwise uniform block of porous matrix. Figure 1 details the system configuration and provides material dimensions and hydrogeologic parameters used in the simulations. There are four system components: the matrix, the fracture, the fracture coating, and the fracture fill. The domain was discretized such

that a thin coating layer could be assigned along the walls of the fracture, between the fracture and matrix. No reported values for actual coating thicknesses were available for assigning thicknesses in the model. Although the thickness of the coating layer was intended to be representative of a real coating, it was also driven by limitations in discretizing the domain for the FEM model. Thus resultant effective coating thicknesses were, perhaps, greater than what might be observed. For simulations where no coating was present the fracture coating elements were assigned matrix properties to maintain a constant fracture aperture for all simulations. Fracture fill could be emplaced by redefining the material characteristics in a given portion of the fracture to those of the fill material. Each part of the system was assigned hydrologic properties and initial saturations based on one of the two fractured systems considered.

The matrix characteristics used in this study represent tuff properties from a heavily welded Topopah Spring tuff from Yucca Mountain (tuff A) and a nonwelded Bandelier tuff from Los Alamos (tuff B). These systems were selected because of their importance to potential or active waste disposal sites, as well as for availability of data. We have run these two tuffs because they have somewhat different hydrologic properties, allowing some sensitivity analysis. The tuff A system follows the physical configuration and material parameters used by *Nitao* [1991]. The tuff B is heavily fractured, with a reported average fracture spacing of 2 m. Parameters for the tuff B system were from measured values [*Rogers and Gallaher*, 1995]. Tuff A capillarity is significantly greater (2–3 orders of magnitude) than that of tuff B, while tuff B porosity and permeability are much higher than those of tuff A.

Since we are explicitly concerned with the fracture in this study, we must be able to distinguish the fracture and explicitly track the flow therein. When using a standard Darcian, finite element porous media simulator, the options of how to represent the fracture are quite limited. With a FEM/FDM (finite difference method) model the fracture nodes/elements must be characterized as porous media and assigned corresponding hydrologic properties (porosity, permeability, etc.), as opposed to explicitly characterizing fracture aperture. In this study, specific "fracture elements" were assigned distinct hydrologic properties. The fracture properties were of a highly porous (95%) and highly conductive ($7.2e^{-03}$ m/s) material (following *Nitao* [1991]). Fracture parameters were selected for high conductivity and low capillarity, reflecting characteristics of an actual fracture and capturing the difference between fracture and matrix behavior within the flexibility of the numerical technique.

Fracture coatings and fracture fills were assigned different properties in the two different tuffs. In tuff B, coatings and fills were assigned clay properties, consistent with field observations [*Davenport*, 1995] showing that coatings consisted of smectites or calcium carbonate. Because we were unable to find any reported hydrologic properties for smectites or carbonates, we chose parameters of a generic clay from the literature [*Mualem*, 1978]. Although a van Genuchten characteristic curve for this generic clay may not be the same as what would be measured for smectite, the actual swelling behavior of the clay is not captured in this model, regardless. Tuff A fracture coatings were assigned the same material parameters as the tuff A matrix except for the saturated hydraulic conductivity, which was reduced. The matrix-like coating is representative of a coating caused by weathering of the matrix or transport of crushed matrix material into the fracture. Figure 1 contains values for the hydrologic properties used for the different material components of the systems.

External boundaries of the modeling domain had no-flow conditions except for the two ends of the fracture. Water was introduced into the top of the fracture, while the bottom of the fracture was open for outflow of water and air. At Los Alamos the water table is more than 200 m below the fractured tuff units of concern and does not influence the hydrology of the system. At Yucca Mountain the Topopah Spring unit varies in distance from the water table; however, we are not concerned here about the influence of the water table on the system, which is an additional issue to be addressed at another time. The domain lengths were sufficiently long to ensure that the bottom boundary conditions did not affect the downward fluid migration.

Two different inflow conditions were applied at the top of the fracture: a constant influx boundary condition (IBC) and a ponded boundary condition (PBC). The IBC represents infiltration during rainfall events, stormwater runoff, or a potential source from an overlying unit. For the tuff A system we used the influx rates reported by *Nitao* [1991]. For the tuff B system we chose an inflow rate based on estimating an "extreme" influx event for LANL, which is discussed in more detail in section 3.2. The PBC represents infiltration from snowmelt and other surface ponding or some other fixed pressure source. The PBC was imposed by applying a source of water at a fixed head along the top of the fracture for 0.5 days and then removing the source.

The simulations were run using the Finite Element Heat and Mass Transfer Code (FEHM) [*Zyvoloski et al.*, 1995]. FEHM is a multidimensional, multiphase, unsaturated and saturated, transient FEM code. FEHM allows different conceptual models for fractures, including dual permeability, dual porosity, and equivalent continuum. For the simple system defined in this work we do not need many of the extensive capabilities of FEHM, but it allows us to continue with studies that will incorporate more complex processes without changing computer codes. The important capabilities of FEHM for this work are its robust handling of sharp interfaces, extreme capillarities, and extreme saturation conditions.

FEHM requires the following hydrologic properties as input: porosity (n), saturated hydraulic conductivity (K_{sat}), and the parameters that define the characteristic curves ($S-\psi$, $k_r-\psi$). We use a *van Genuchten* [1980] curve fit model to represent the constitutive relationships, which requires two parameters, α and N, given in Figure 1. The van Genuchten α is representative of the air entry pressure for the material, while N represents the slope of the soil-water retention curve. Note that K_{sat} of the coatings and fills was the only material property that was not fixed in the simulations presented here. Variation of the van Genuchten parameters was beyond the scope of the work reported here.

Using the single fracture system described above, we ran a series of simulations to identify the effects of different system conditions/configurations on fluid movement between the fracture and matrix. Values of different parameters were varied to test the sensitivity of the fracture-matrix interactions for a range of potentially existing configurations. The characteristics that were varied include (1) presence, absence, and continuity of a fracture coating, and saturated hydraulic conductivity (K_{sat}) of that coating; (2) presence or absence of fill in the fractures, location along and length in the fracture, and K_{sat} of

Table 1. Values Used for Parameters Being Varied in the Simulations

Parameter	Range of Values
	Tuff A Parameters
Inflow condition cm/day	$q_l = 0.011$, $q_m = 0.11$, $q_h = 1.1$
K_{sat} (coating), m/s	no coating; $1.7e^{-13}$, $1.7e^{-15}$, $1.7e^{-17}$
Initial matrix saturation	0.15, 0.40, 0.65, 0.95
	Tuff B Parameters
Inflow condition	2.5 cm/d flux rate, 0.5 day ponded
K_{sat} (coating), m/s	no coating; $9.5e^{-09}$, $9.5e^{-11}$
Coating continuity	continuous; 2-m gap at $y = -5$ m, 0.20-m gap every 1 m to $y = -10$ m
K_{sat} (fill), m/s	no fill; $1.09e^{-15}$, $1.09e^{-17}$
Fill length	no fill; 2 m, 10 m
Fill location	no fill; $y = 0$ m, $y = -2$ m

Here y is the vertical direction, with $y = 0$ at the top of the system.

the fill; (3) combinations of fill and coating conditions; (4) initial matrix saturation; (5) influx rate under constant influx conditions; and (6) the flux (IBC) versus ponded (PBC) inflow condition. Table 1 shows the range of values run for the different parameters. Combinations of the various parameters were selected as appropriate for the various simulations.

3. Observations

In this section we present observations from the simulations. For simplicity we have divided this section into subsections based on tuff A or tuff B. Discussion of the implications of the observations to physical systems, as well as comparisons of simulations from the tuff A versus the tuff B systems, are found in section 4.

3.1. Tuff A Fracture-Matrix System

For the tuff A configuration, sensitivity to three parameters was tested: initial matrix saturation, fracture wall coating conductivity, and water inflow rate. The uncoated fracture system was used as the basis for comparison for the various simulations. We also used these simulations to check our results against those reported by *Nitao* [1991], which used a different porous media simulator. The results from FEHM agreed almost exactly with Nitao's reported values. These simulations showed the fracture-dominated versus matrix-dominated behavior that occurs at high versus low flow rates, respectively, at early times. This system reached a matrix dominated flow regime in approximately 10 days at the q_m (see Table 1), long before the water reached the bottom of the system. Thus most of the displacement occurred with a relatively flat invading front and predominantly matrix flow.

The first set of comparisons considered the role of coating conductivity in the tuff A system. For these simulations the initial matrix saturation was 0.15 and the flux rate was equal to q_m (Table 1). Figure 2 shows the fluid distributions in the system at $t = 46.3$ days for each of four coating conductivities used, as given in Table 1. The saturation profile for the uncoated fracture (Figure 2a) is orthogonal to the fracture. The matrix and fracture are in capillary equilibrium and their respective fronts move together. A fracture coating with a K_{sat} only 2 orders of magnitude (O(2)) smaller than that of the matrix (Figure 2b) did not strongly affect the ability of the matrix to imbibe the water moving in the fracture. The effect of this O(2) coating layer was to increase the depth of water infiltration in the fracture, slightly increase the depth of water penetration in the matrix, and slightly decrease the saturation in the matrix behind the front at a given time. Thus the presence of this coating effectively spread the water through more of the matrix but did not channel the flow in the fracture. For these two cases (Figures 2a and 2b) the system remained in a basically matrix-dominated regime, with lateral flow through the matrix occurring over a very short time frame and most of the flow in the matrix occurring as a flat, vertical front.

When the fracture coating K_{sat} was O(4) smaller than that of the matrix (Figure 2c), most of the flow became channeled in the fracture. However, particularly in this lower initial saturation system, the matrix was still able to imbibe approximately 25% of the liquid flowing into the system. In this case the system remained in a regime with matrix flow dominated by lateral movement out from the fracture. The lateral penetration of liquid into the matrix was fairly uniform with depth. The saturation in the matrix remained fairly low, and the lateral velocity of the front was relatively small.

By the time the fracture coating K_{sat} was O(6) below that of the matrix (Figure 2d), virtually all imbibition from fracture to matrix was eliminated. In this case, the matrix only imbibed on the order of 1–3% of the liquid that was transported through the system. For this low conductivity coating, the fracture truly became a "fast path" for flow.

The set of simulations with different coating conductivities was repeated for four different initial matrix saturations: 0.15, 0.40, 0.65, and 0.95. Figure 2, and the discussion above, represent the system with an initial matrix saturation of 0.15. For the higher initial saturations the overall trends in behavior were similar to those observed in the 0.15 saturated case. There were two major differences between runs at different initial saturations. The first was a decrease in ratio of matrix K_{sat} to coating K_{sat} necessary to cause channeled fracture flow. This change results from the decrease in matric capillary suction that occurs with increased matric saturation. For initial matrix saturations of 0.65 and 0.95, a O(4) difference between matrix and fracture conductivity was sufficient to cause most of the liquid to remain in the fracture.

The second effect of initial matrix saturation was a decrease in the amount of time before water flowed primarily in the fracture. For the 0.95 saturation, which is near the in situ saturation of tuff A, the base case simulation proceeded similarly to the uniform front seen in Figure 2a with a slight increase in the penetration depth near the fracture. For the O(2) coating the wetting front proceeded like that shown in Figure 2b but was more disperse. Even at this high initial saturation, matrix imbibition slowed the advancement of the wetting front. We should note that as saturation increases, the time required to saturate the matrix block decreases. For example, at an initial matrix saturation of 0.15, it took 150 days to saturate the matrix, while at 0.95 saturation it took only approximately 10 days. This is consistent with the amount of time that would be required to saturate the matrix volume at the designated inflow rate. Once the matrix block saturated, the fracture began to act as a conduit.

Finally, these simulations were repeated for three different inflow rates: q_h (fracture dominated), q_m (intermediate), and q_l (matrix dominated). Here the inflow rate, q, is the effective infiltration rate for the entire upper boundary, but the water is injected only into the fracture. These rates represent extreme flow for Yucca Mountain, where net infiltration is estimated to be less than 5 mm/yr [*Montazar and Wilson*, 1984]. The results

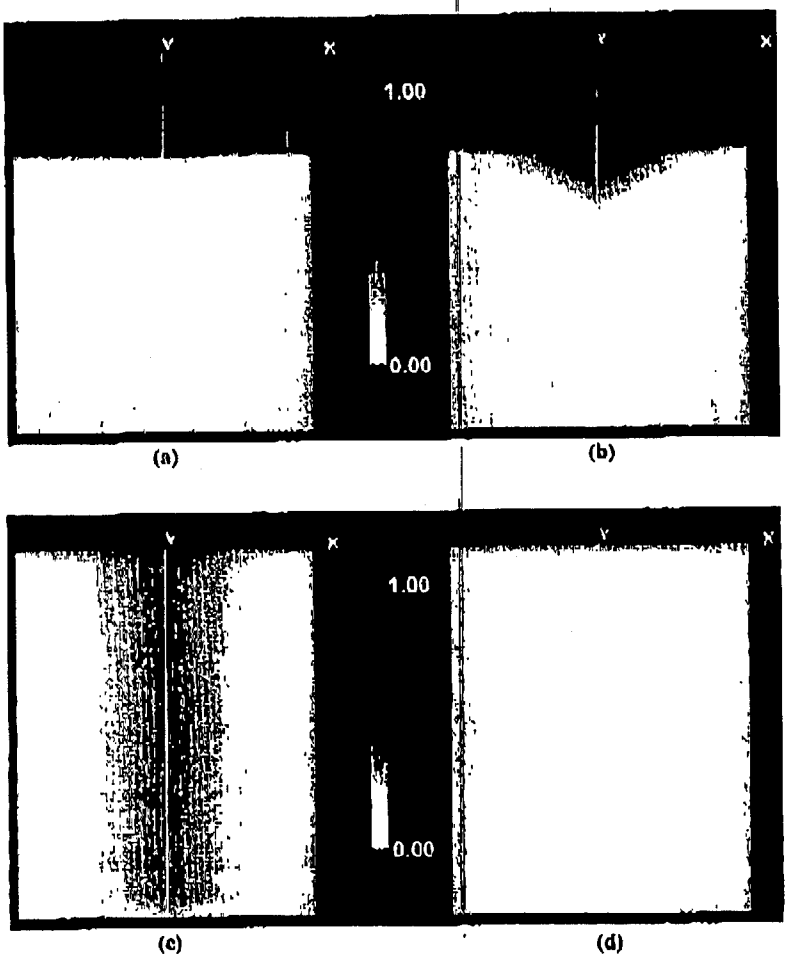


Figure 2. Effect of coating conductivity on infiltration and fracture-matrix interaction in tuff A. Time = 46.3 days. K_{sat}(coating): (a) no coating (K_{sat}(matrix)), (b) $1.7e^{-13}$ ($10^{-2} \times K_{sat}$(matrix)), (c) $1.7e^{-15}$ ($10^{-4} \times K_{sat}$(matrix)), and (d) $1.7e^{-17}$ ($10^{-6} \times K_{sat}$(matrix)).

from this series of simulations were not sensitive to the injection rate used except in terms of the time required to saturate the system. Although some variation in the overall characteristics of the liquid front was observed for different injection rates, the variation was consistent between changes in initial matrix saturations and coating K_{sat}.

3.2. Tuff B Fracture-Matrix System

The remaining simulations presented here were done in the tuff B fracture-matrix system. All simulations were run with a 0.05 initial matrix saturation, which is the average measured in situ saturation for the specific physical system represented [*Rogers and Gallaher*, 1995]. The tuff layer represented here is one layer of mesa stratigraphy, on a mesa that is approximately 3 km long and 0.5 km wide. The tuff unit lies 12 m below the mesa surface and approximately 250 m above the water table. The extremely low in situ saturation is attributed to evaporation through fractures and volcanic surge beds that are open to the atmosphere.

Two different top fracture boundary conditions were applied for the tuff B single fracture runs. In one set of simulations the IBC was applied, while in another set of simulations the PBC was applied. In the IBC simulations $q \approx 2.5$ cm/d was applied continuously for the duration of the runs. This influx rate is considered to be an extreme influx condition for the native arid environment. Locally, annual precipitation is only 36 cm and net infiltration is estimated to be less than 10 mm/yr [*Birdsell et al.*, 1997]. In PBC simulations the top of the fracture was held at saturation for 0.5 days. After 0.5 days the fixed saturation was replaced with a no-flow condition, eliminating the introduction of additional water. Water already in the system at t = 0.5 days was allowed to redistribute or flow out. Note that the effective inflow rate for this ponded condition was generally more than an order of magnitude larger than the IBC rate, generating conditions that fell within a fracture dominated regime.

As with the tuff A our basis for comparison of the tuff B sensitivity runs was the simple matrix-fracture system with no coating and no fill. For this configuration, regardless of the top boundary condition, all of the water entering the system was rapidly imbibed into the matrix, resulting in matrix and fracture front velocities that were approximately equal. The characteristic of the invading front was not significantly different from that occurring in a system without a fracture and with point injection at the surface. There was a time period when the infiltrating water moved both laterally and vertically, which was on the order of 10 days for the IBC system and 1 day for the PBC. Following that period, the water moved downward

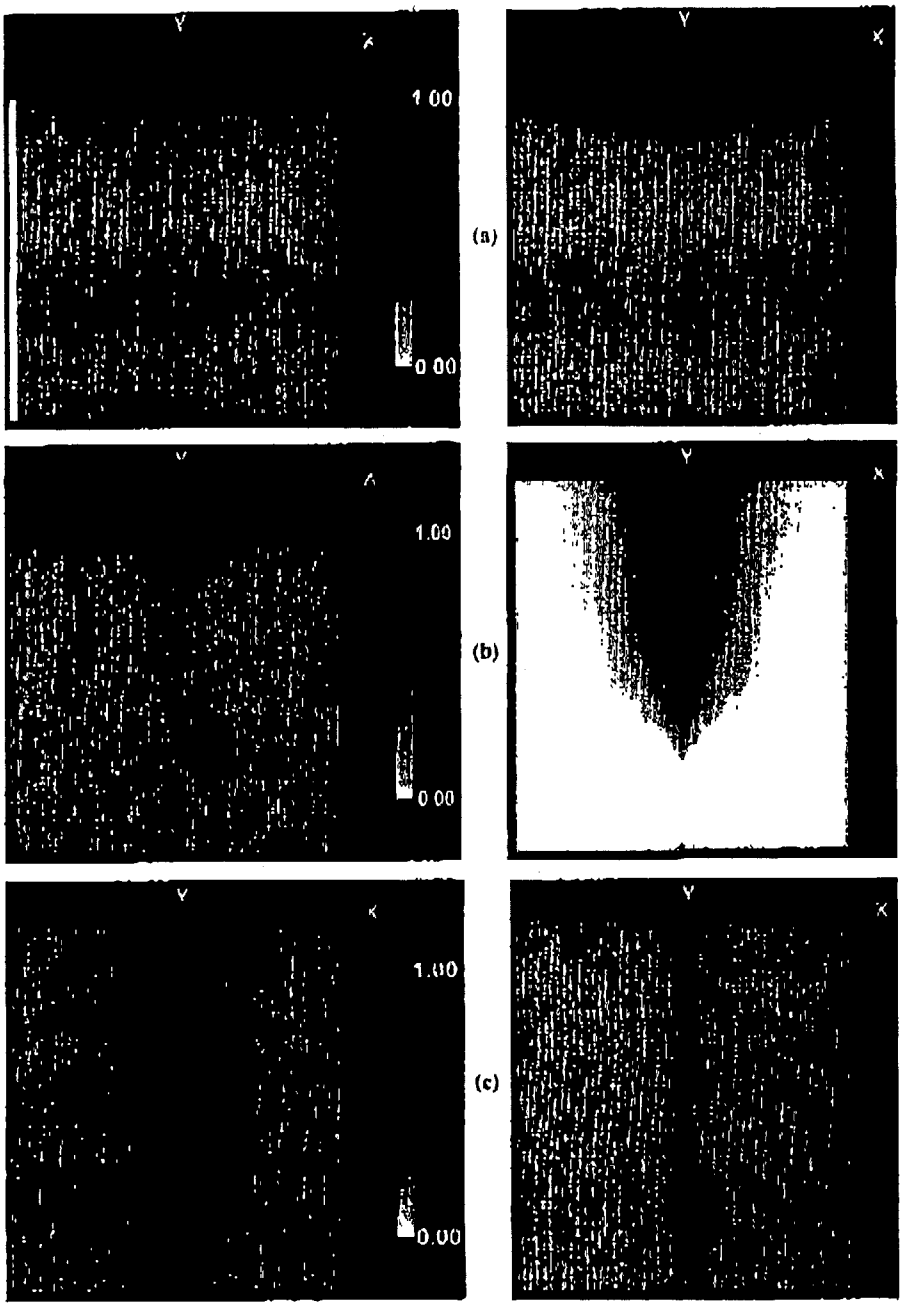


Figure 3. Effect of coating conductivity on infiltration and fracture-matrix interaction in tuff B. Left column is the IBC at t = 25 days. Right column is the PBC at t = 0.5 days. K_{sat}(coating): (a) no coating (K_{sat}(matrix)), (b) clay ($\sim 10^{-2} \times K_{sat}$(matrix)), (c) modified clay ($\sim 10^{-4} \times K_{sat}$(matrix)).

with a uniform, horizontal front, with no apparent influence of the fracture.

The first series of simulations assessed the effect of changing the coating hydraulic conductivity on the resulting water flow. The results of these simulations for tuff B are consistent with those from tuff A. Figure 3 shows the results for the three different coatings for the two inflow boundary conditions. Note the difference in timescales for these different conditions. We observe that the effect of a coating along the walls of the fracture is dependent on the relative conductivities of the coating and the matrix. In Figure 3b the conductivity of the clay used for the coating material here is only O(2) lower than that of the matrix. This coating did little to prevent liquid in the fracture from being imbibed by the matrix. However, the reduced conductivity did cause an increase in the vertical depth the water traveled down the system. As the coating conductivity was decreased further (Figure 3c), the flow was increasingly channeled in the fracture. When K_{sat} of the clay was decreased by 10^{-2}, (O(4) lower than the matrix, and hereinafter called "modified clay"), flow was predominantly in the fracture; however, the matrix did imbibe water over time, more or less uniformly over the length of the fracture. Most of the matrix imbibition, however, was at later times, well after the water in the fracture started exiting the bottom of the domain. One reason for this might be that the injection rate was greater than the outflow rate allowed by the bottom boundary condition. In

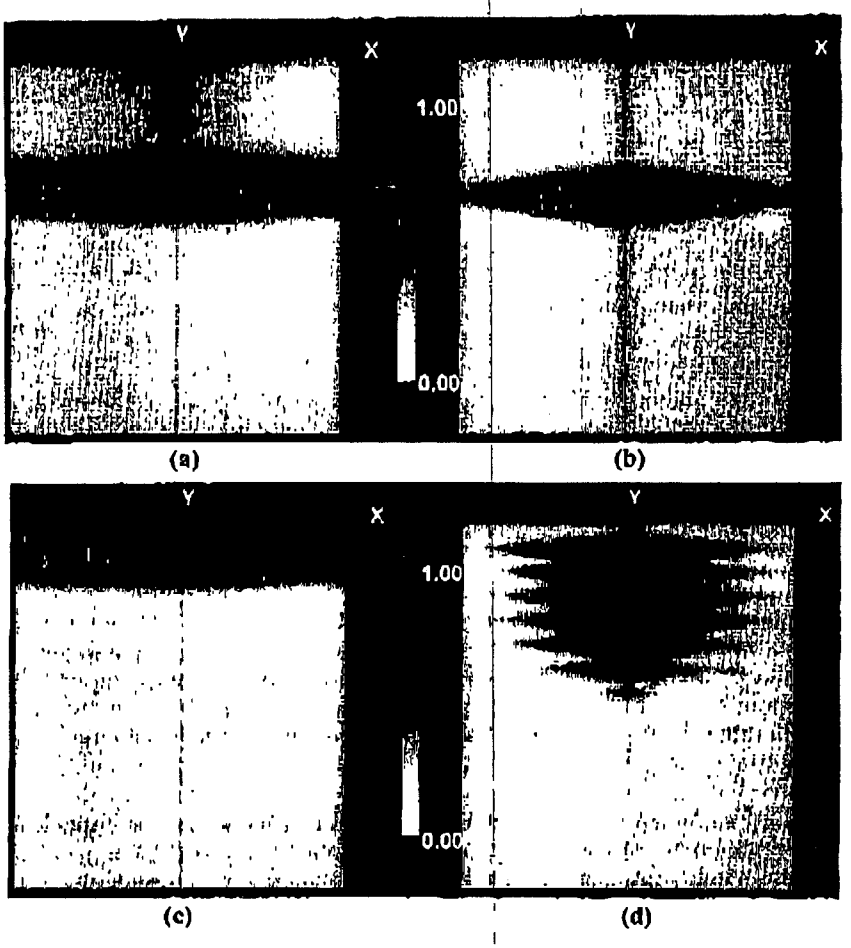


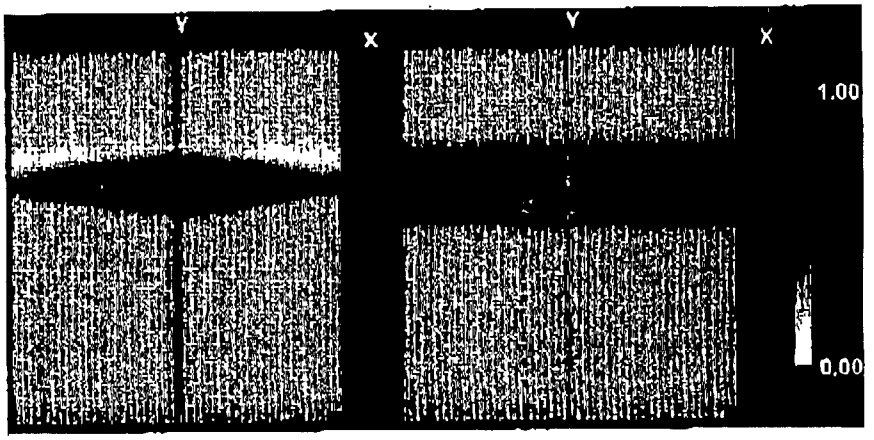
Figure 4. Effect of fracture coating discontinuity on infiltration and fracture-matrix interaction in tuff B. Left column is the IBC at $t = 25$ days. Right column is the PBC at $t = 0.5$ days. ((a), (b)) Single 2-m discontinuity at $y = -5$ m and ((c), (d)) 0.2-m discontinuity every 1 m starting at $y = -1$ m.

the ponded simulation once the liquid source was removed (after 0.5 days) all of the liquid in the fracture was rapidly imbibed into the matrix, and the liquid in the matrix spread until it appeared to reach an almost uniform saturation above the penetrating front.

Figure 3 shows an increase in the depth of the leading edge of the liquid front depending on the rate at which water entered the system. For the IBC the difference was initially great, but by 25 days it was almost unnoticeable. The high initial inflow rate of the PBC resulted in a more fracture-dominated system and a steeper wetting front. The ponded case with fracture coatings produced penetration distances of the liquid front that were more than twice that of the uncoated case.

In the second series of simulations we introduced discontinuities into the coating layer. For all of these simulations we used the modified clay conductivity to minimize liquid entering the matrix through the coating. Two different cases were run: (1) a single gap between 5 and 7 m below the surface and (2) a series of short (0.2 m) discontinuities every meter starting at 1 m below the surface (Table 1). Figure 4 compares the two coating conditions for the two boundary conditions. For the IBC injection the break in coating effectively halted the movement of water down the fracture (Figures 4a and 4c). This behavior was observed for both the small, intermittent discontinuities as well as for the single gap. For the IBC case all of the injected water was apparently able to enter the matrix at the first discontinuity, and further downward movement occurred only in the matrix. The saturation in the coating increased to approximately 0.8 along the entire length of the fracture but the saturation in the fracture itself remained under 0.3.

Under the PBC condition, water also rapidly entered the breaks in the coating, but the downward movement of water in the fracture was not halted (Figures 4b and 4d). The difference in response was due to the high effective inflow rate for PBC, which caused the matrix around the coating discontinuities to saturate very rapidly. As the matrix saturation increases, the capillarity drops significantly, and the rate at which the water moves laterally in the matrix, away from the fracture, versus the rate at which it flows past the gap in the coating decreases. Thus more water was available to continue down the fracture. Ahead of the front there was no increase in saturation, even in the coating layer. This behavior was less significant in the IBC case because the rate of lateral flow in the matrix remained greater than the rate of downward flow in the fracture. In neither case, however, was there any water outflow at the bottom of the fracture. Note also, for the PBC, once the water source was removed the water in the system was rapidly imbibed by the matrix and redistributed to eliminate major saturation gradients. Figure 5 shows the effect of removal of the water source with the PBC condition. In none of the simulations with a discontinuous coating did any water reach the bottom of the fracture.



(a) (b)

Figure 5. Fluid distribution in the tuff B system for the PBC and a discontinuous coating just before and after the source of water is removed: (a) t = 0.5 days, (b) t = 10.0 days.

The final series of simulations analyzed the importance of fracture fill. This was studied by placing a fill in the fracture and varying its length and location. Simulations were run with the top of the fill at two locations: even with the top of the system (y = 0 m) and 2 m below the surface (see Table 1), and two lengths of fill, 2 and 10 m. Unless otherwise noted, the fracture fill was assigned modified clay parameters. In all cases where the fill was located at the top of the system, it acted as an effective barrier to the penetration of water into the system. The saturation of the fill material itself increased, but no water entered the fracture below the fill. Instead, the water effectively ponded above the fracture until the pressure buildup caused the solution not to converge. When the fill was located below the surface, the response depended on the presence, absence, and conductivity of a fracture coating layer. With no fracture coating the fill provided a barrier to flow in the fracture, but the water moved unimpeded through the matrix. When the standard clay coating was imposed the system responded identically to the uncoated condition. For the modified clay conductivity the water saturated the fracture above the fill and did not infiltrate any further. The system response was the same regardless of inflow condition or fill length.

4. Discussion and Implications

What do these simulations tell us about fracture flow in permeable matrix systems and about tuff systems specifically? In this section we consider what the observations tell us in terms of fractures as fast flow paths, increased depth of the infiltration front, influence of coating discontinuities, role of fracture fills, and limitations of the modeling approach. Further, we postulate what behavior can be anticipated if we consider the role of cyclic evaporation and infiltration events, which was not included in the simulations reported here.

The most dominant observation from the simulations was that in almost every case, the fractures were not a priori a "fast flow path" for water. Even during extremely high infiltration events when no coatings or fills were present, fractures in these tuff systems were not able to carry water very far. At the influx rates used, there were only a few conditions under which we observed liquid traveling the entire length of the system. When there was a significant (4 orders of magnitude or greater) and continuous reduction in conductivity at the fracture-matrix interface, water was found to be strongly channeled in the fracture. Also, when the initial matrix saturation was very high, less time was required before the fracture began to flow (corresponding to reduced time to saturate the matrix). Although these results indicate that fractures are unlikely to play a dominant role in moving water from the surface to the water table in low-saturation high-capillarity systems, there are reasonable natural conditions that are sufficient to produce significant flows. High influx conditions (similar to our PBC) that may cause water to move a significant distance in a fractured system include rapid snowmelt, large runoff events, or areas with the potential for ponding. Highly saturated systems may also produce significant fracture flow, although they must be subject to sufficient inflow.

Lower K_{sat} coatings were not able to eliminate matrix imbibition; however, reduced conductivity did allow water to penetrate deeper into the fracture-matrix system during an infiltration event. The repercussions of spreading the infiltration front deeper is that the increase in saturation in the matrix near the fracture acts to decrease the capillarity drawing water into the matrix. The increased saturation also increases the conductivity of the matrix to water. These two results produce conditions that allow water to penetrate deeper into the system.

The results of these simulations are generally consistent with laboratory observations. *Thoma et al.* [1992] found that in a tuff sample with visible coating there was a substantial (10^{-7}) reduction in the effective permeability of the sample but that with no visible coating the decrease in the effective permeability between a natural fracture and a freshly broken sample was quite small (0.3). *Chekuri et al.* [1995] observed slightly increased imbibition into coated samples of Tiva Canyon tuff over fresh surfaces. For the Topopah Spring tuff they observed decreased imbibition into coated surfaces which they could model by decreasing the sample permeability by a factor of $\frac{1}{2}$.

The simulations presented here represent only a single infiltration event. The system response to short cycle time, high-infiltration events is still unknown. Do multiple short cycles produce more or less flow in the fracture and matrix? In a scenario of repeated infiltration events, water entering the system at each subsequent event would tend to travel further down the fracture (less loss to matrix), and water in the matrix would also move faster (higher conductivity). Under this sce-

nario we could envision the fractures enhancing downward movement. However, if there is significant time between infiltration events, during which the fractures act as conduits for evaporation, the presence of the fractures may enhance evaporative loss from the matrix. The evaporation would remove the water that infiltrated during the infiltration event, negating its effects. Under this scenario the fractures could potentially reduce effective infiltration. These questions remain to be addressed in appropriate studies.

When fracture-matrix interaction is reduced by a coating, the system remains in a fracture-dominated flow regime for a longer period of time and water is able to infiltrate deeper into the system before being imbibed by the matrix. The increased saturation in the matrix near the fracture faces after an infiltration event could provide a higher conductivity flow path for the following infiltration event, given that the next event occurs before the system dries out. Partial fracture coatings also aid in increased infiltration depth. However inflow rates and water volumes must be high enough to exceed the matrix capillarity.

We observed that discontinuities in the low-conductivity coatings on the fracture walls interrupted fast flow down the fracture. The high capillarity of the tuffs suggests that a break in any fracture coating will allow water to rapidly enter the matrix. A discontinuity in a surface coating of 20 cm was sufficient to strongly reduce the amount of water in the fracture in these simulations. However, for the extreme, effective influx rate of the PBC a few short discontinuities were not sufficient to eliminate flow in the fracture. The water was able to penetrate almost 10 m during the half day over which water was available to the system.

On the basis of these observations we anticipate that the observed fluid behavior will be sensitive, to some extent, to the size of the gaps in the coating. The size of the coating gap used here was mainly based on the discretization of the system. However, few measurements of coating extent are available. Those measurements that have been reported indicate high variability in coating condition, from sparse to almost none, to relatively dense with small cracks [*Carlos et al.*, 1995; *Chekuri et al.*, 1995]. Discontinuities resulting from shrinkage and swelling of clay coatings are expected to be quite small. These discontinuities might not provide sufficient exposed matrix area to eliminate fracture flow. The region of the matrix around such a small gap would rapidly become saturated and strongly reduce the lateral flow of water into the matrix. The extent to which the size of the gap will result in fracture dominated flow is unknown. Further simulations with finer gaps must be run in the future to identify the dependence of extent of matrix imbibition on discontinuity size.

When we consider the role of fills in affecting water infiltration, the results are quite consistent. Fractures that are filled at the exposed surface of the fracture are effective barriers to inflow into the fracture. However, if the matrix next to the fracture reaches saturation, water might trickle into the fracture as with a seepage face. The importance or extent of such seepage is unknown at this time, but it is not expected to result in significant fracture flow in itself.

Fills below the surface are also effective barriers to continuous flow down the fracture. With no coating or only minimal conductivity reduction at the fracture wall above the fill, water entering the fracture is readily imbibed into the matrix and proceeds down as matrix flow. When a continuous, low conductivity coating is present the water neither moves into the matrix above the fill nor passes through the fill and into the fracture below, but rather it ponds at the surface. A fracture that ends within a matrix block or at the interface between two blocks will behave like a fracture that is filled at that location. The path for the water in the fracture is eliminated, and the water must find an alternate route through the subsurface. This means that even if a fracture provides a "fast path" for water through part of the system, it is also necessary for it to be continuous down to the elevation of interest for that path to be of major concern.

Although the matrix materials were limited to tuffs in the simulations presented in section 3, we believe that the results can be generalized to some extent. The lack of sensitivity of the overall trends to variations in many of the parameters supports some generality of the conclusions. For example, we observed that the general trend of decreasing matrix imbibition with decreasing coating conductivity was consistent at all initial matrix saturations. We observed that for the tuff B system, which has a lower matrix capillarity, less difference between matrix K_{sat} and coating K_{sat} was required to decrease matrix imbibition. We would thus anticipate that a matrix material of weaker capillarity (higher van Genuchten α) than those simulated here would respond similarly to the simulations run at higher initial matrix saturations (e.g., wetting fronts would move more quickly through the system, and less decrease in coating permeability is required to induce fracture flow). We have also observed similar infiltration patterns for two different coating materials with somewhat different hydrologic properties. This by no means provides justification to extrapolate to any coating material, but does provide some confidence for a range of coating materials. Part of the effort in the continuation of this work will be sensitivity studies for different matrix, coating/fill, and fracture characteristics.

5. Summary and Conclusions

This study has presented a first step in better understanding fracture flow in unsaturated, high-capillarity porous media and provides some guidelines for directing future field, laboratory, and modeling studies. In this paper we assessed the role of fracture coatings and fracture fills in modifying flow in fractures. Using a domain consisting of a single fracture embedded in a permeable porous matrix, we studied the effect of different observed fracture features on flow in fractures and flow between the fractures and matrix. We considered existence and continuity of coatings and fills as well as the role of initial matrix saturation and infiltration conditions. Within the regime studied in this work, it was determined that fractures are unlikely to provide rapid, open channels for flow. Only under certain conditions are fractures in high-capillarity, low-saturation environments the primary flow path. When there is significant reduction in conductivity (communication) between the fracture and the matrix along the entire length of the fracture and relatively large volumes of water entering the fracture, the infiltrating water remains in the fracture. High initial matrix saturations also lead to more rapid fracture-dominated flow. However, intermittent coatings, even covering 80% of the fracture surface, are not sufficient to eliminate significant matrix imbibition. Fracture flow is also virtually eliminated when the fracture is plugged for even a short length, by fill material. The most likely role of fractures is to increase the depth that liquids penetrate during cyclic infiltration events, a premise that remains to be tested.

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